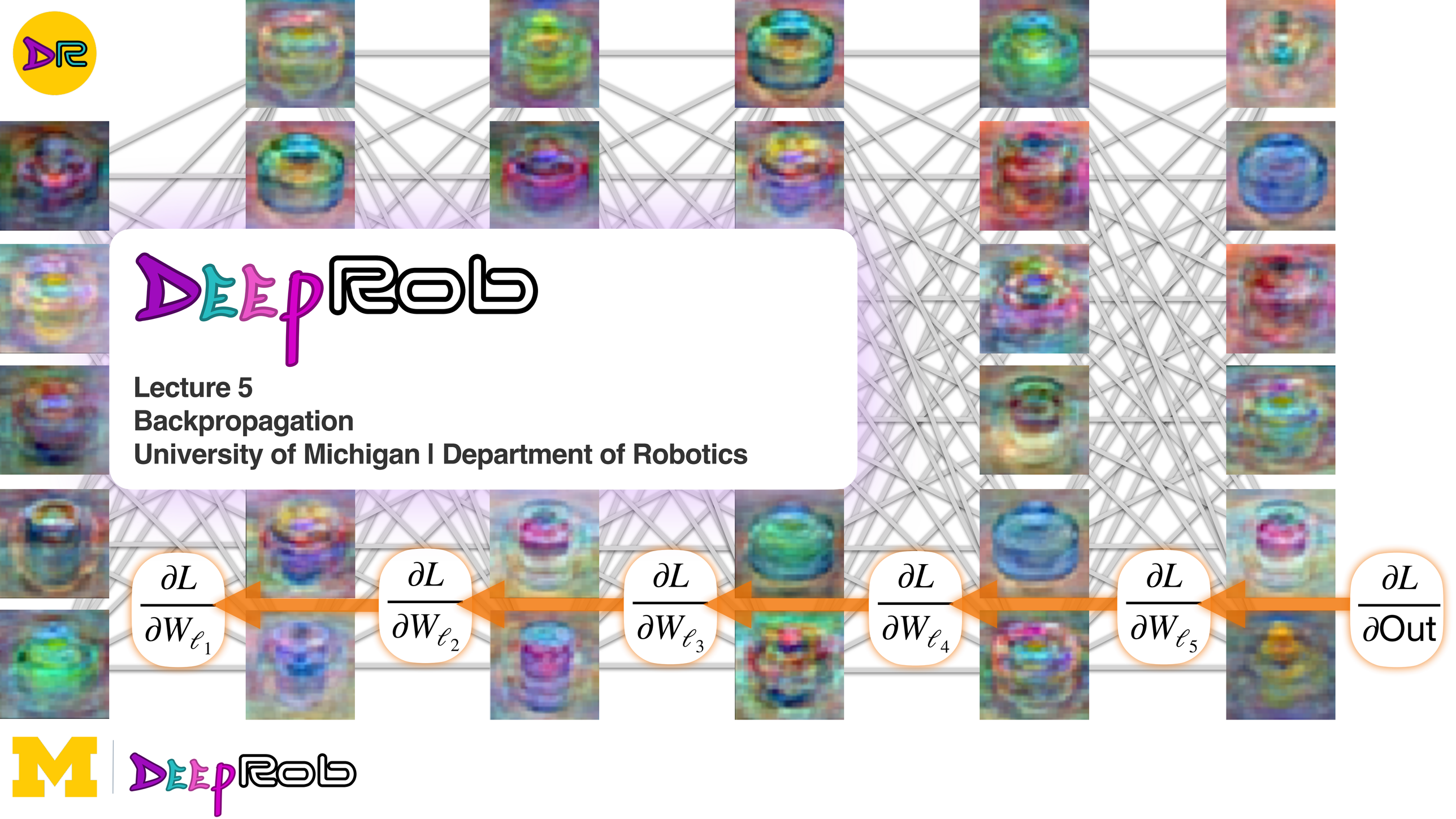
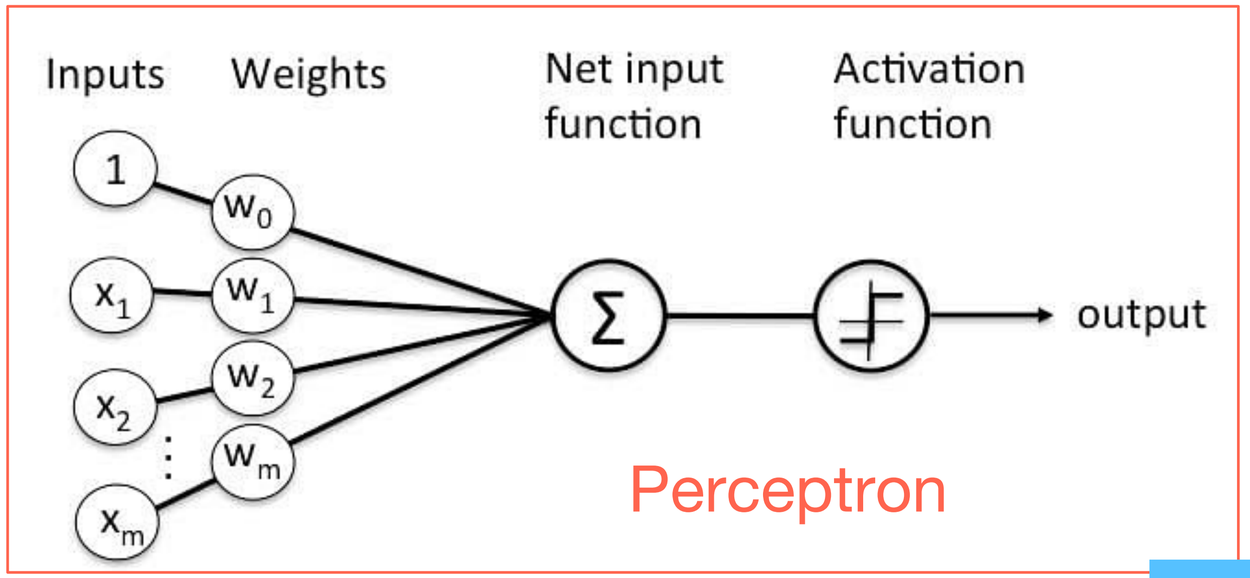

DEEPROB
Lecture 5
Backpropagation
University of Michigan | Department of Robotics
$\frac{\partial L}{\partial W_{\ell_1}}$
$\frac{\partial L}{\partial W_{\ell_2}}$
$\frac{\partial L}{\partial W_{\ell_3}}$
$\frac{\partial L}{\partial W_{\ell_4}}$
$\frac{\partial L}{\partial W_{\ell_5}}$
$\frac{\partial L}{\partial \text{Out}}$
DEEPROB

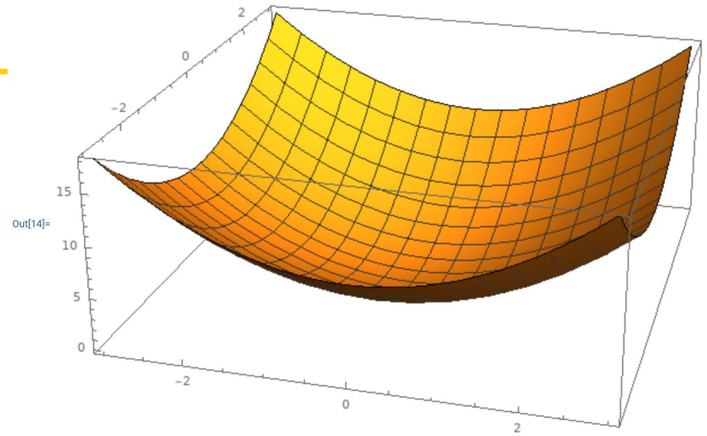
Project 1—Reminder

- Instructions and code available on the website
  - Here: deeprob.org/projects/project1/
- Implement KNN, linear classifier, and fully connected NN
- **Due Thursday, Feb.1, 11:59 PM EST**
- **Late policy: 3 late tokens (24hrs each with no penalty); 25% deduction for every day the submission was late after using all three late tokens**

Recap: Neural Networks

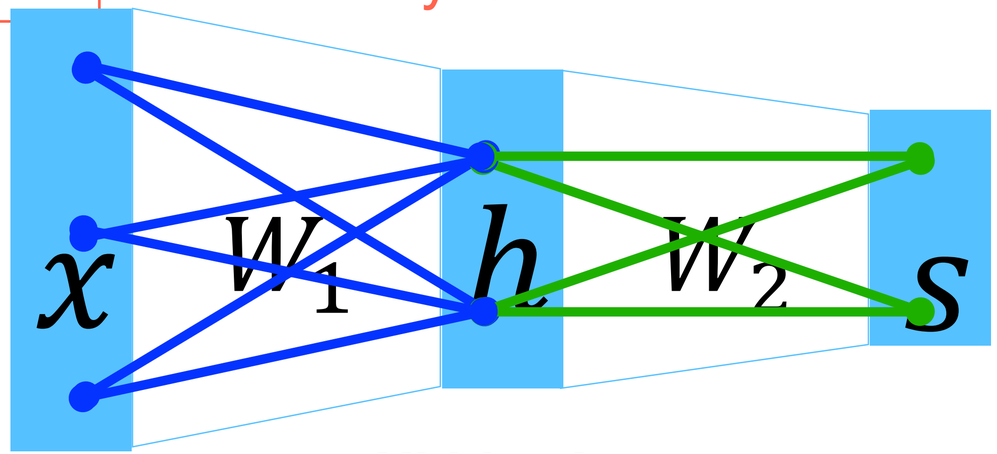


Perceptron



MLP

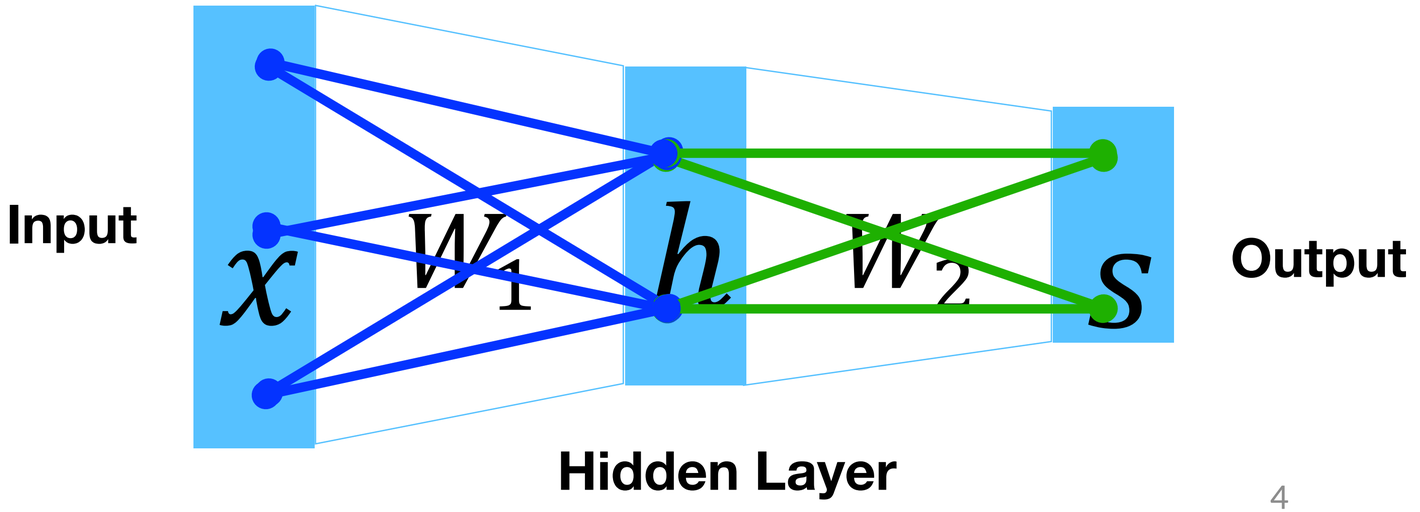
"Fully Connected"



Problem: How to compute gradients?

$$s = W_2 max(0, W_1 x + b_1) + b_2$$

Nonlinear score function



Problem: How to compute gradients?

$$s = W_2 max(0, W_1 x + b_1) + b_2$$ Nonlinear score function

$$L_i = \sum_{j \neq y_i} max(0, s_j - s_{y_i} + 1)$$ Per-element data loss

$$R(W) = \sum_k W_k^2$$ L2 regularization

$$L(W_1, W_2, b_1, b_2) = \frac{1}{N} \sum_{i=1}^{N} L_i + \lambda R(W_1) + \lambda R(W_2)$$ Total loss

If we can compute $\frac{\delta L}{\delta W_1}, \frac{\delta L}{\delta W_2}, \frac{\delta L}{\delta b_1}, \frac{\delta L}{\delta b_2}$ then we can optimize with SGD

(Bad) Idea: Derive $\nabla_W L$ on paper

$$s = f(x; W) = Wx$$

$$L_i = \sum_{j \neq y_i} max(0, s_j - s_{y_i} + 1)$$

$$= \sum_{j \neq y_i} max(0, W_{j,:}x - W_{y_i,:}x + 1)$$

$$L = \frac{1}{N} \sum_{i=1}^{N} L_i + \lambda \sum_k W_k^2$$

$$= \frac{1}{N} \sum_{i=1}^{N} \sum_{j \neq y_i} max(0, W_{j,:}x - W_{y_i,:}x + 1) + \lambda \sum_k W_k^2$$

$$\nabla_W L = \nabla_W \left(\frac{1}{N} \sum_{i=1}^{N} \sum_{j \neq y_i} max(0, W_{j,:}x - W_{y_i,:}x + 1) + \lambda \sum_k W_k^2 \right)$$

Problem: Very tedious with lots of matrix calculus

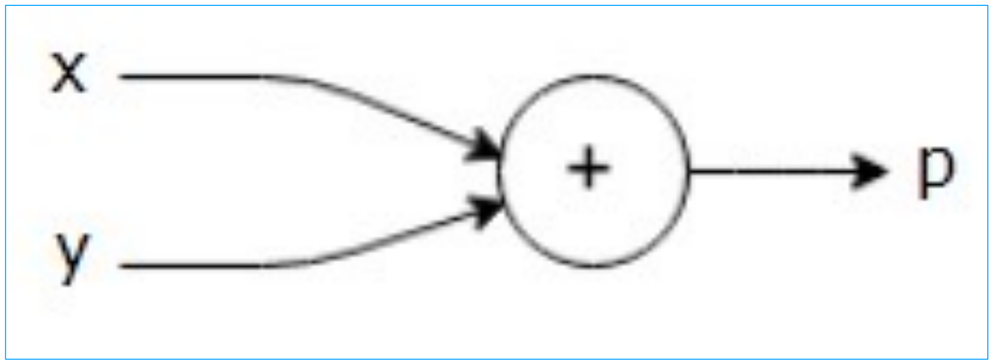
Problem: What if we want to change the loss? E.g. use softmax instead of SVM? Need to re-derive from scratch. Not modular!

Problem: Not feasible for very complex models!

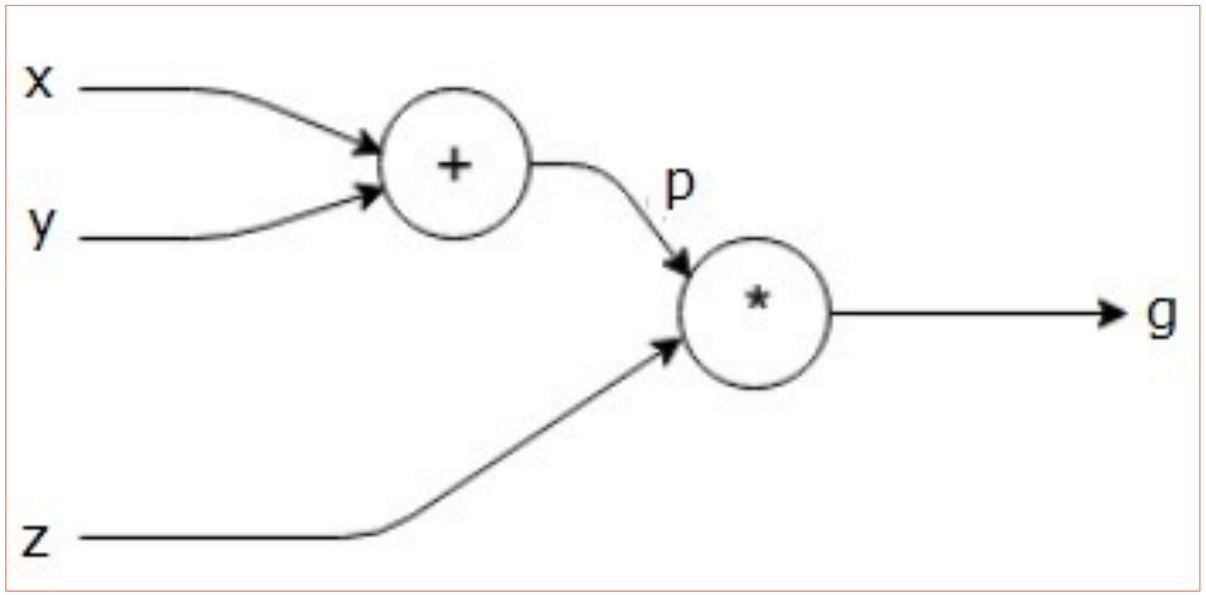
Better Idea: Computational Graphs

Simple example:

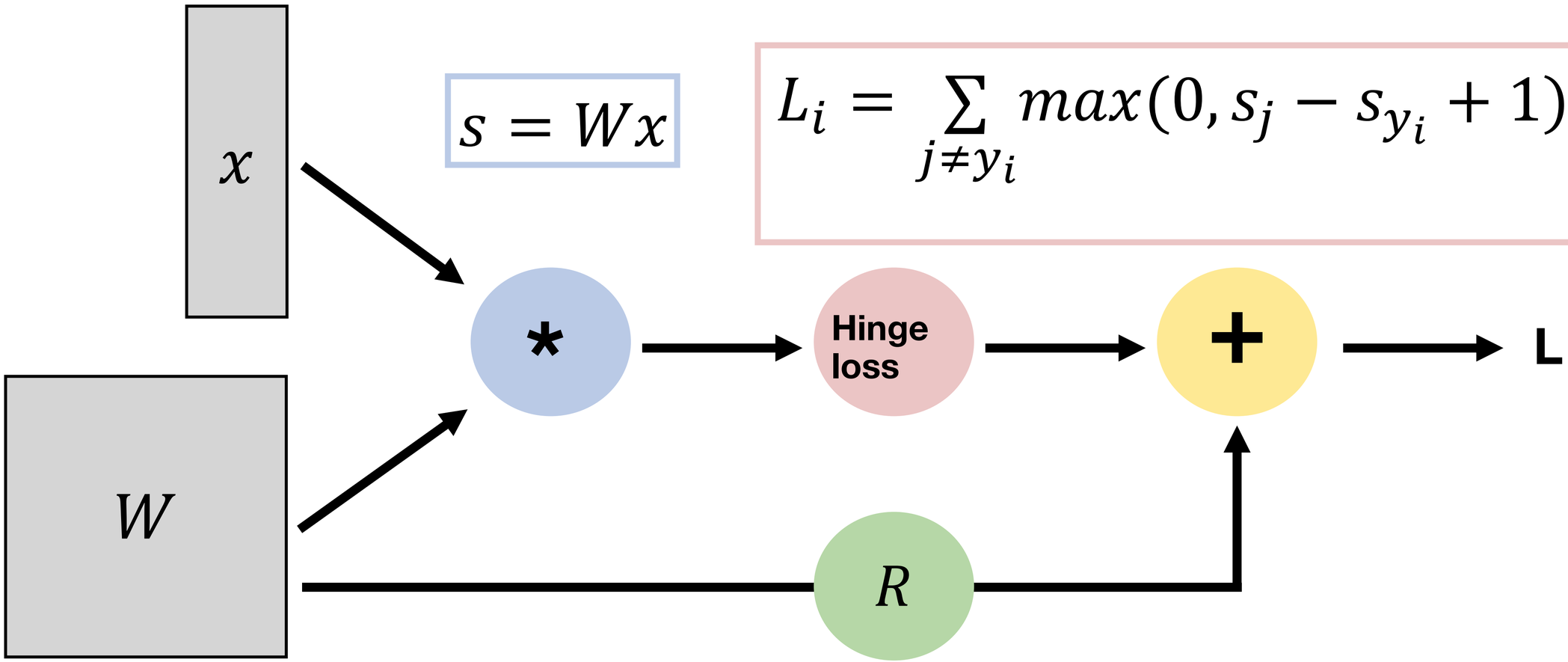
$$p = x + y$$



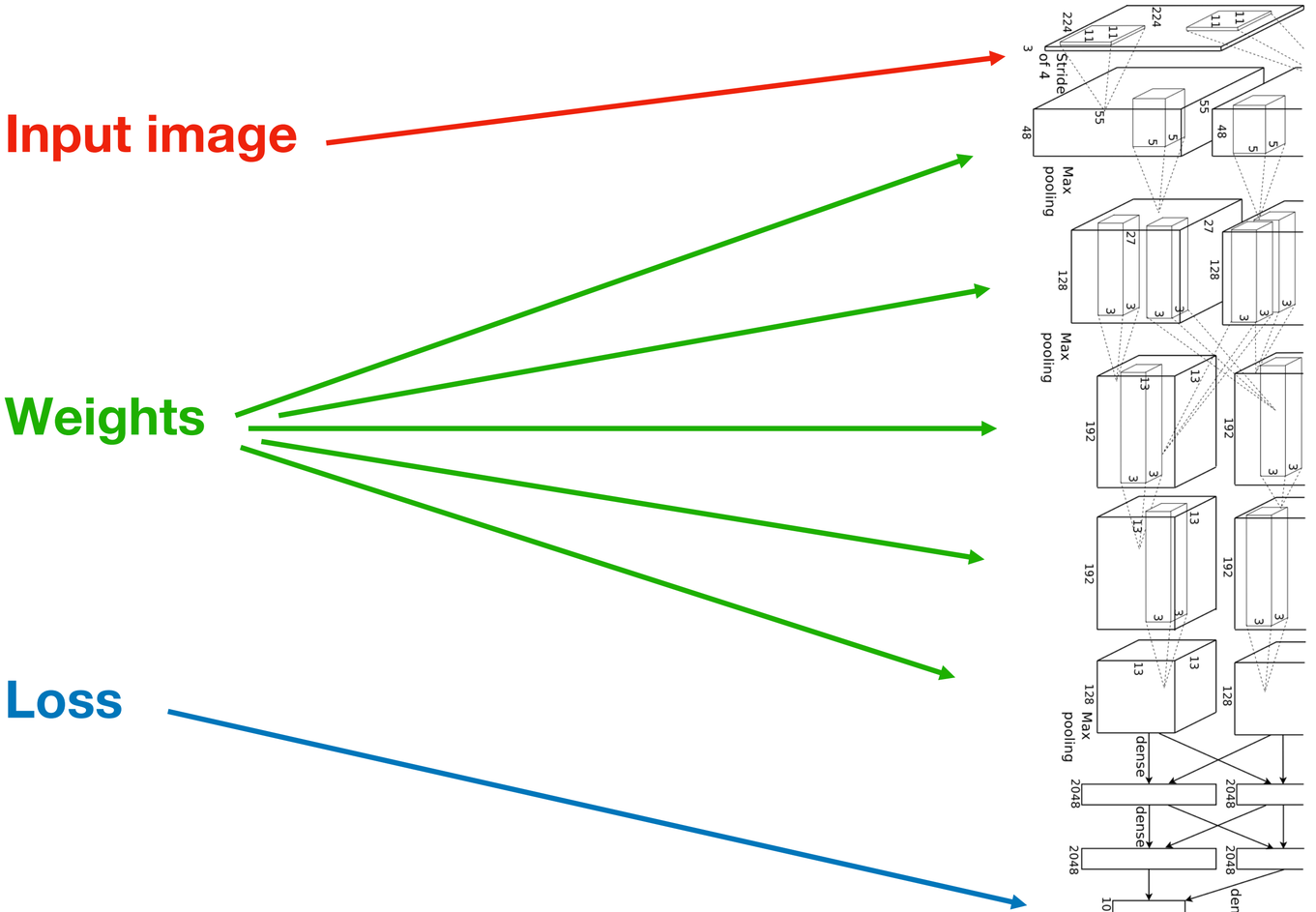
$$p = (x + y) * z$$



Better Idea: Computational Graphs

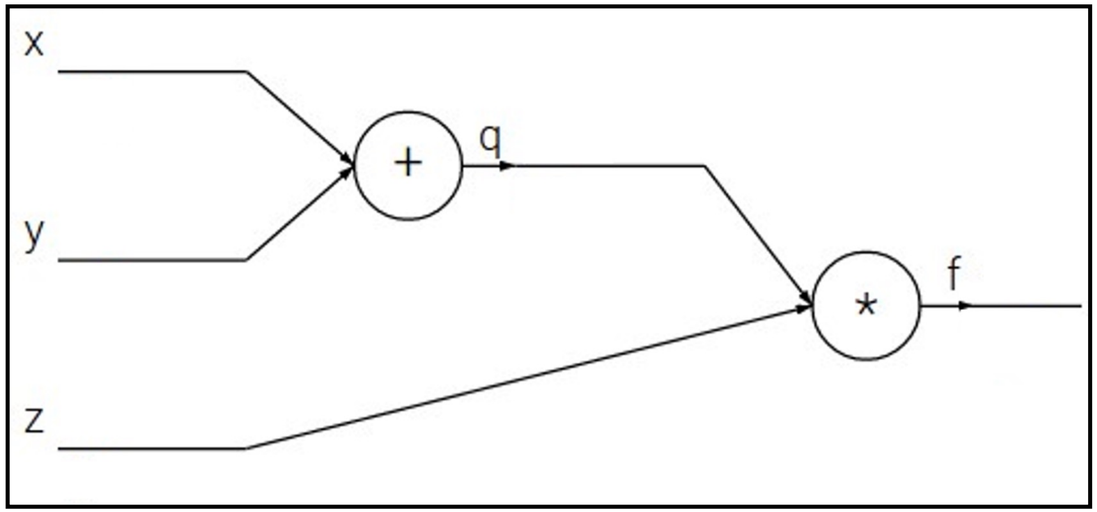


Deep Network (AlexNet)



Backpropagation: Simple Example

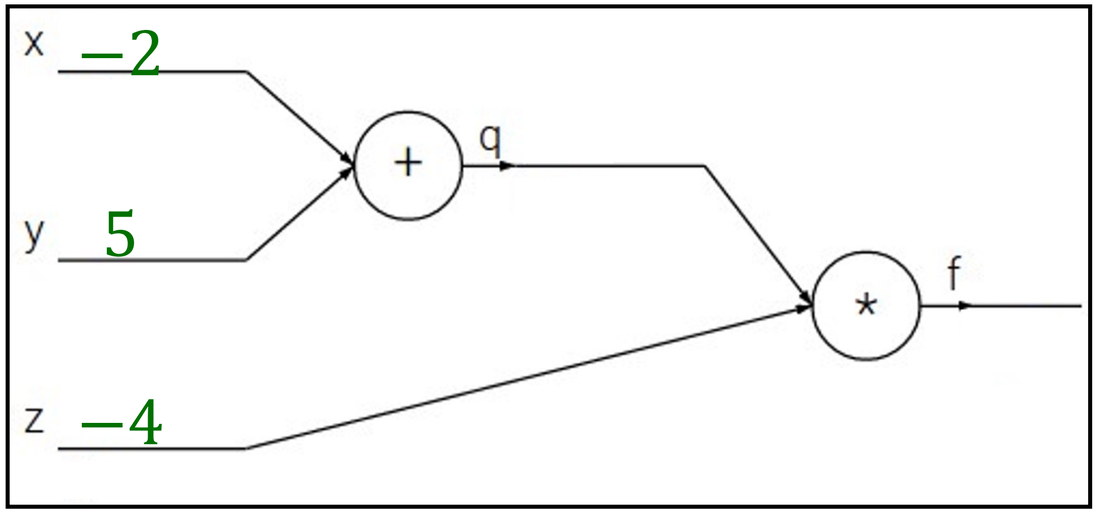
$$f(x, y, z) = (x + y) \cdot z$$



Backpropagation: Simple Example

$$f(x, y, z) = (x + y) \cdot z$$

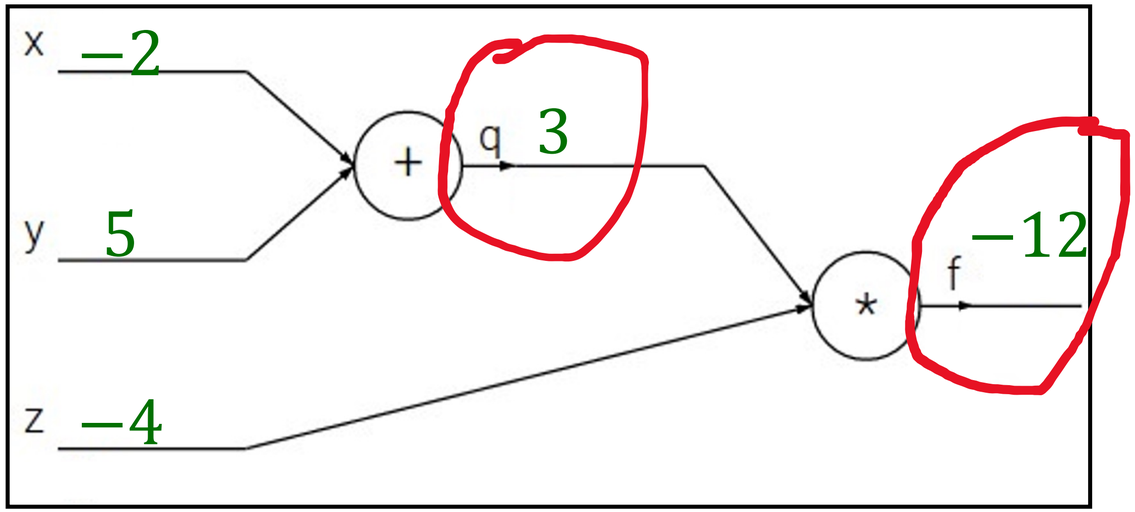
e.g. $x = -2, y = 5, z = -4$



Backpropagation: Forward Pass

$$f(x, y, z) = (x + y) \cdot z$$

e.g. $x = -2, y = 5, z = -4$



1. Forward pass: Compute outputs

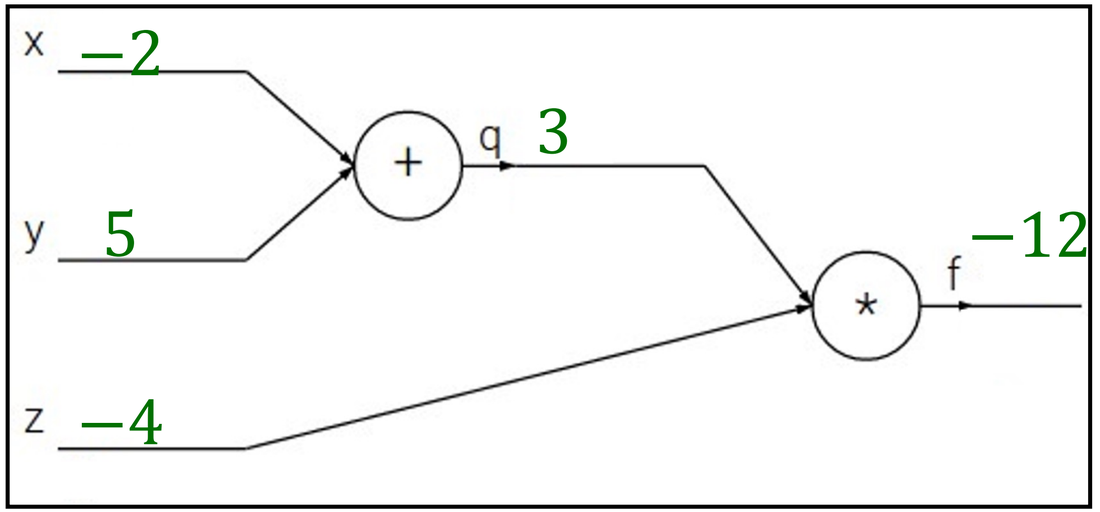
$$q = x + y = -2 + 5 = 3$$

$$f = q \cdot z = 3 * (-4) = -12$$

Backpropagation: Backward Pass

$$f(x, y, z) = (x + y) \cdot z$$

e.g. $x = -2, y = 5, z = -4$



1. **Forward pass**: Compute outputs

$$q = x + y \quad f = q \cdot z$$

2. **Backward pass**: Compute derivatives

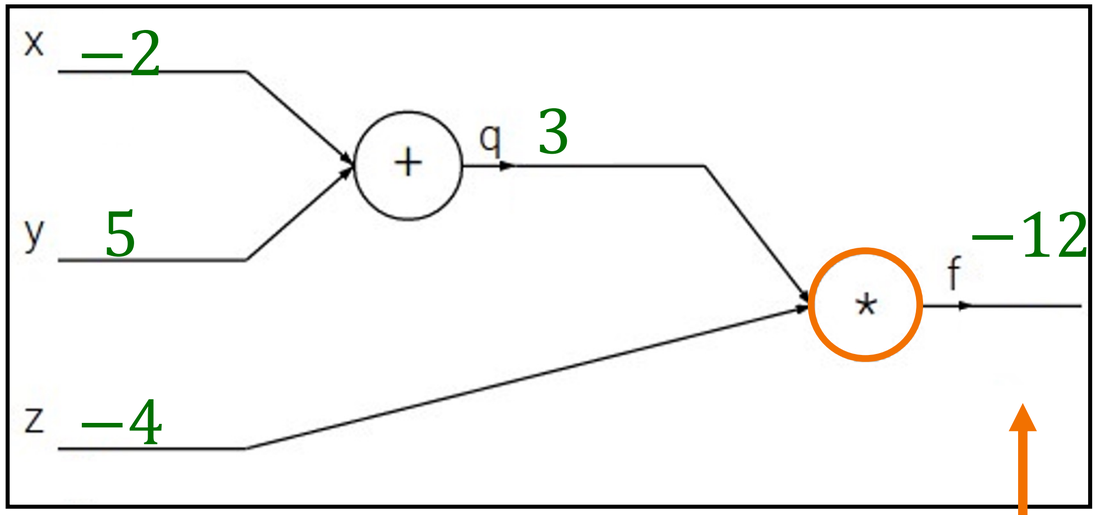
Want: $\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z}$

Problem: What is $\frac{\partial f}{\partial f}$?

Backpropagation: Simple Example

$$f(x, y, z) = (x + y) \cdot z$$

e.g. $x = -2, y = 5, z = -4$



1. Forward pass: Compute outputs

$q = x + y$ $\quad$ $f = q \cdot z$

2. Backward pass: Compute derivatives

Want: $\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z}$

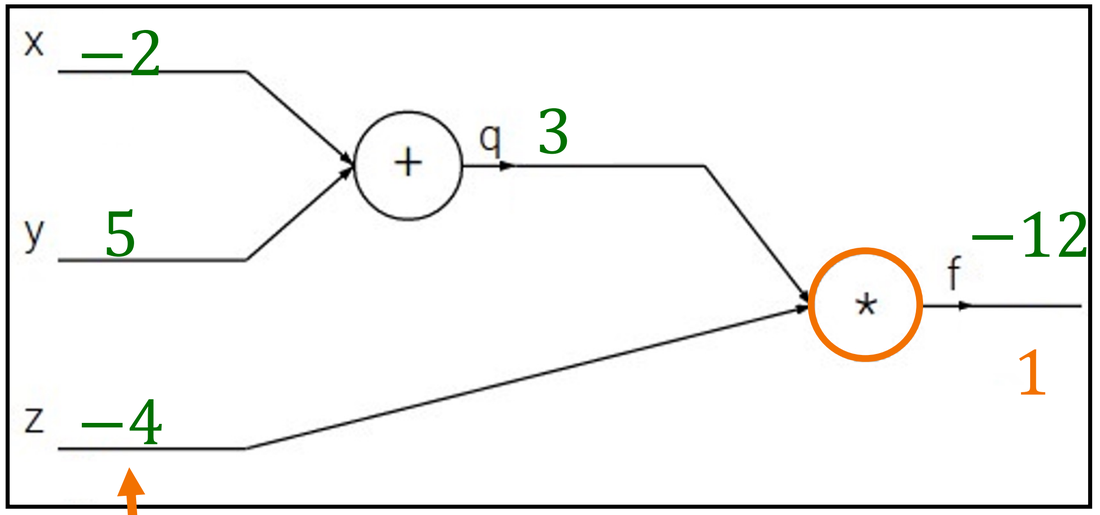
$\frac{\partial f}{\partial f}$

$= 1$

Backpropagation: Simple Example

$$f(x, y, z) = (x + y) \cdot z$$

e.g. $x = -2, y = 5, z = -4$



1. Forward pass: Compute outputs

$q = x + y$ $\quad$ $f = q \cdot z$

2. Backward pass: Compute derivatives

Want: $\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z}$

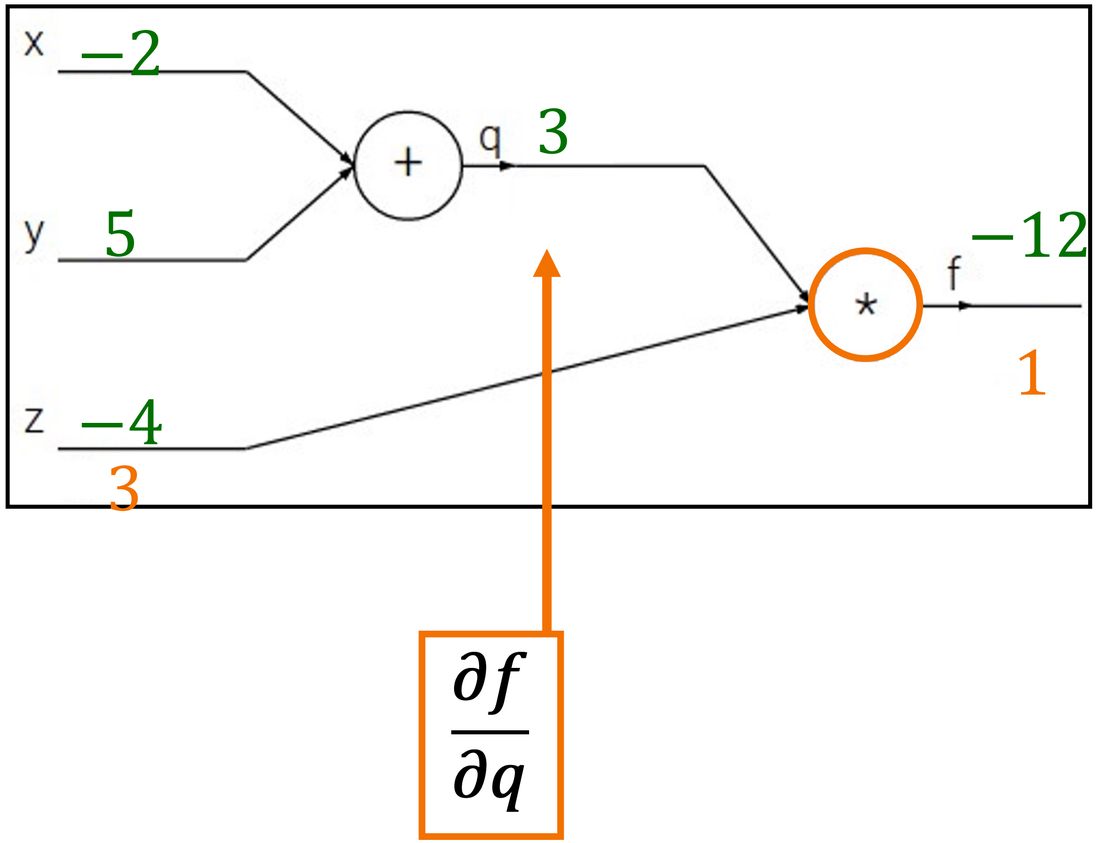
$\frac{\partial f}{\partial z}$

$= q = 3$

Backpropagation: Simple Example

$$f(x, y, z) = (x + y) \cdot z$$

e.g. $x = -2, y = 5, z = -4$



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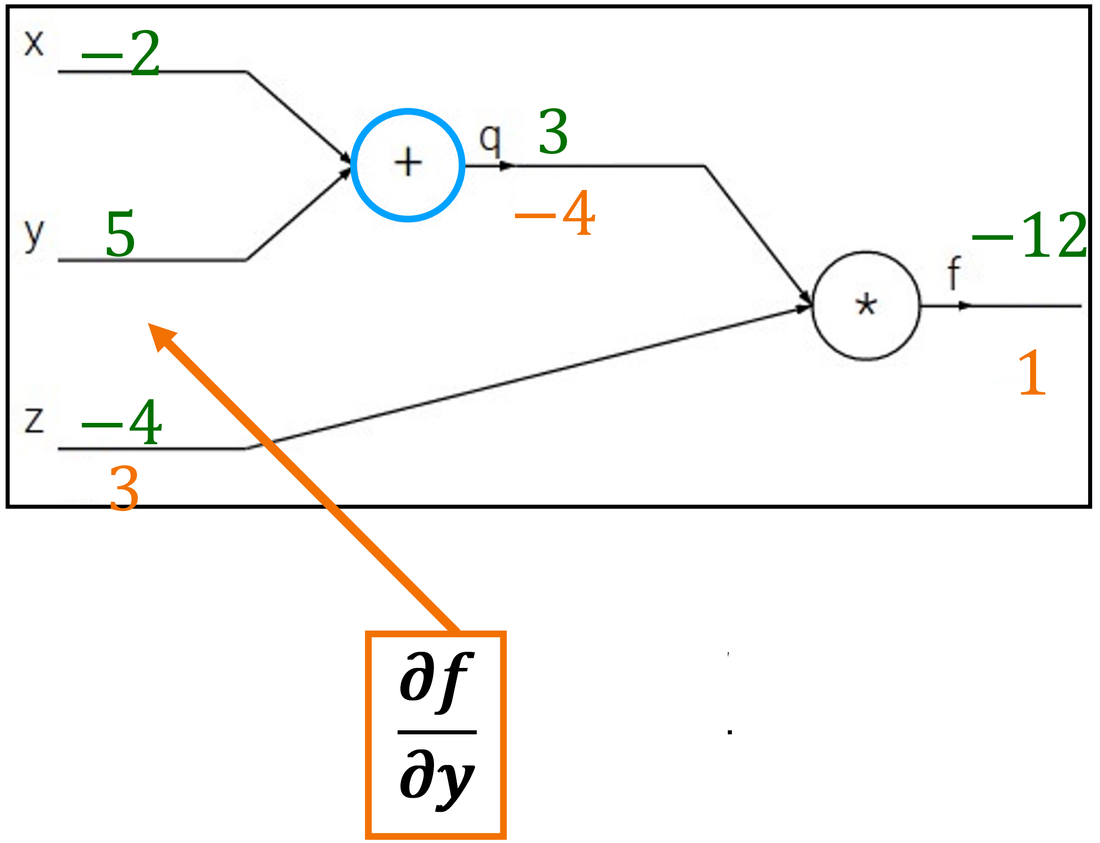

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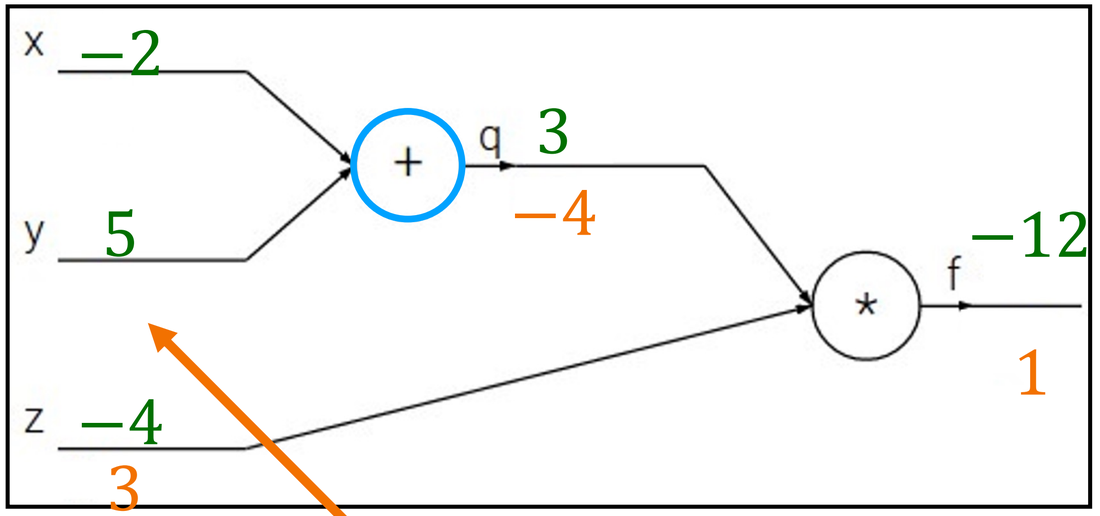

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$$q = x + y \quad f = q \cdot z$$

2. Backward pass: Compute derivatives

Want: $\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z}$

"the chain rule"

$$\frac{\partial f}{\partial y} = \frac{\partial q}{\partial y}\frac{\partial f}{\partial q}$$

Downstream Gradient

Local Gradient

Upstream Gradient

Backpropagation: Simple Example

$$f(x, y, z) = (x + y) \cdot z$$

e.g. $x = -2, y = 5, z = -4$

1. Forward pass: Compute outputs

$$q = x + y \qquad f = q \cdot z$$

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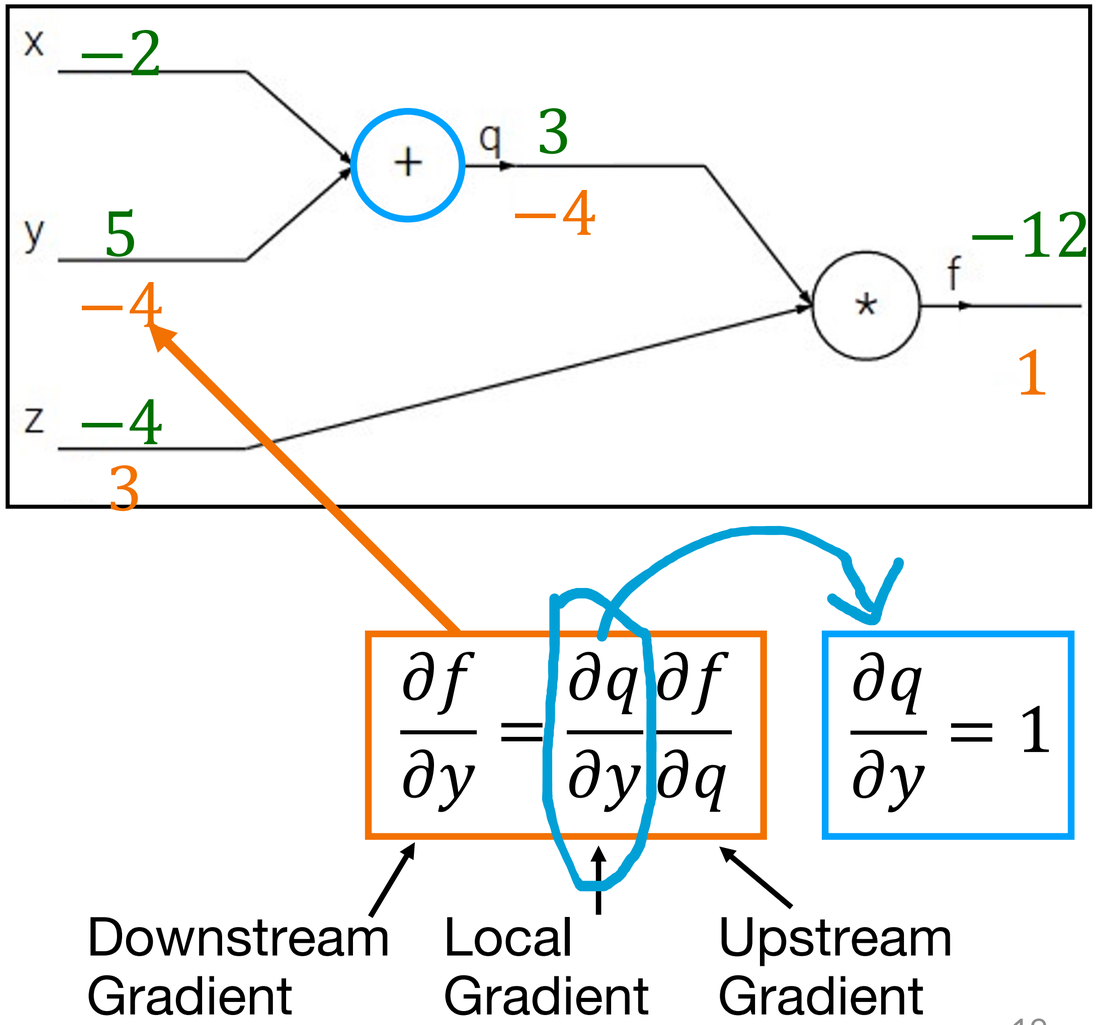

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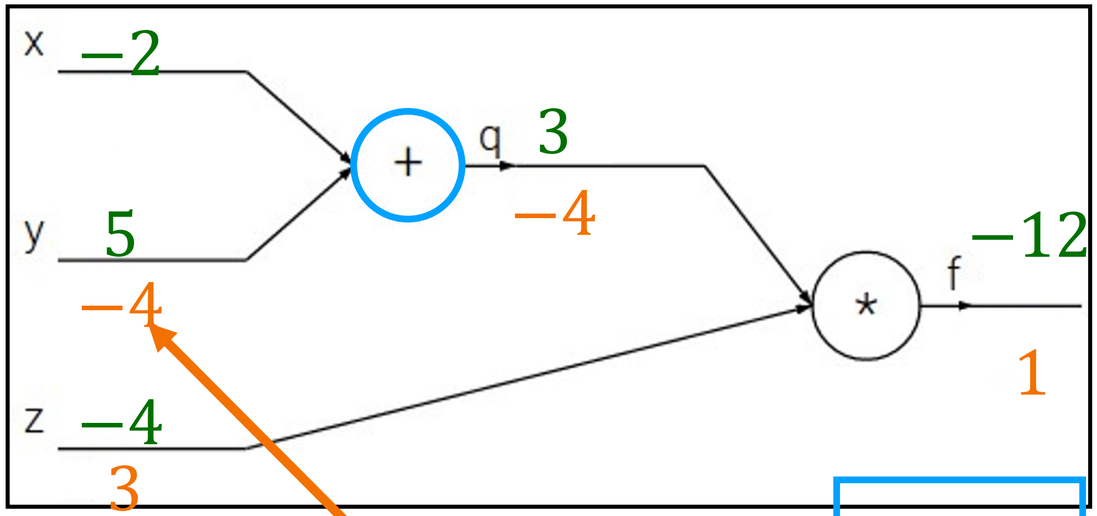
Want: $\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z}$



$$\frac{\partial q}{\partial y} = 1$$

$$\frac{\partial f}{\partial y} = \frac{\partial q}{\partial y}\frac{\partial f}{\partial q}$$

$$\frac{\partial f}{\partial q} = z = -4$$

Downstream Gradient | Local Gradient | Upstream Gradient

Backpropagation: Simple Example

$$f(x, y, z) = (x + y) \cdot z$$

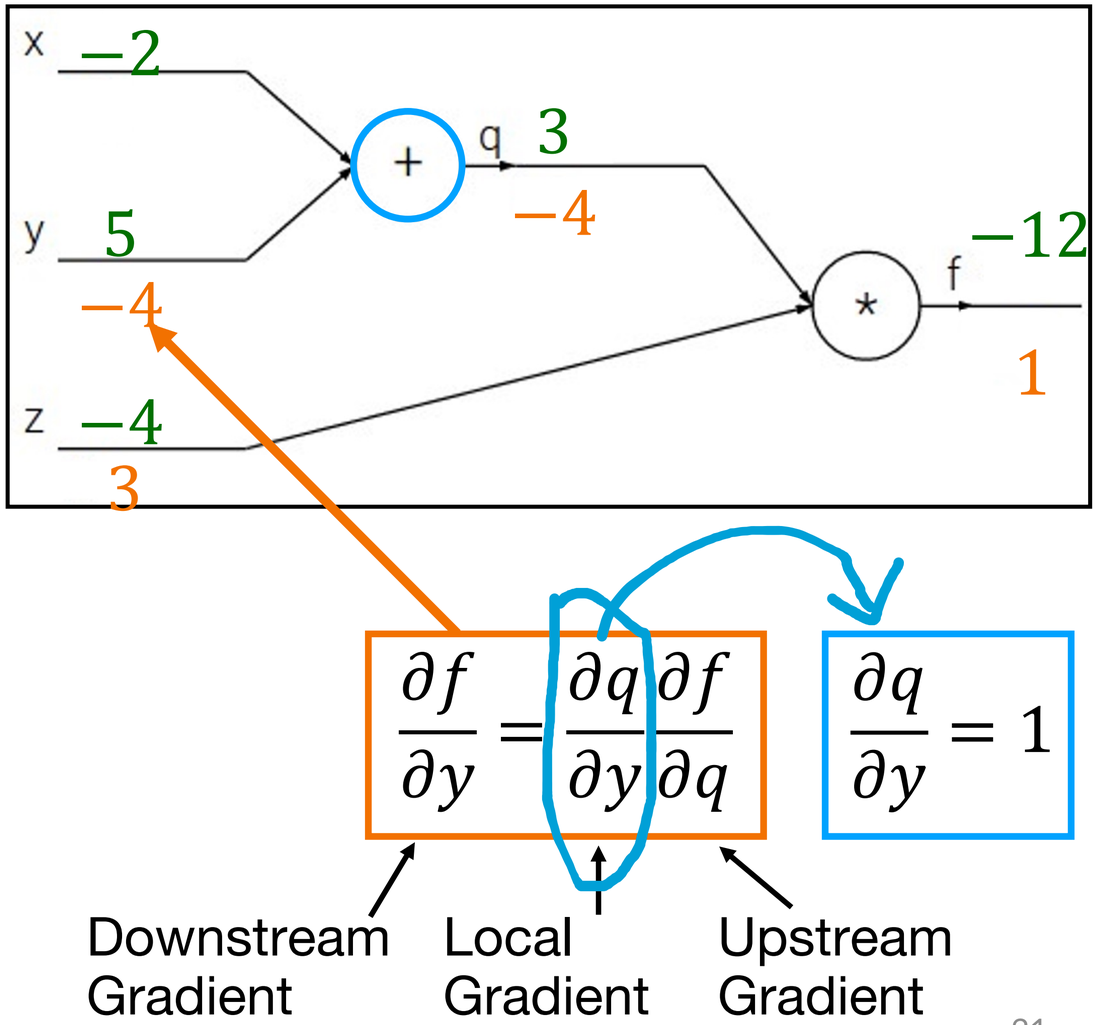
e.g. $x = -2, y = 5, z = -4$

1. Forward pass: Compute outputs

$$q = x + y \qquad f = q \cdot z$$

2. Backward pass: Compute derivatives

Want: $\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z}$



Backpropagation: Simple Example

$$f(x, y, z) = (x + y) \cdot z$$

e.g. $x = -2, y = 5, z = -4$

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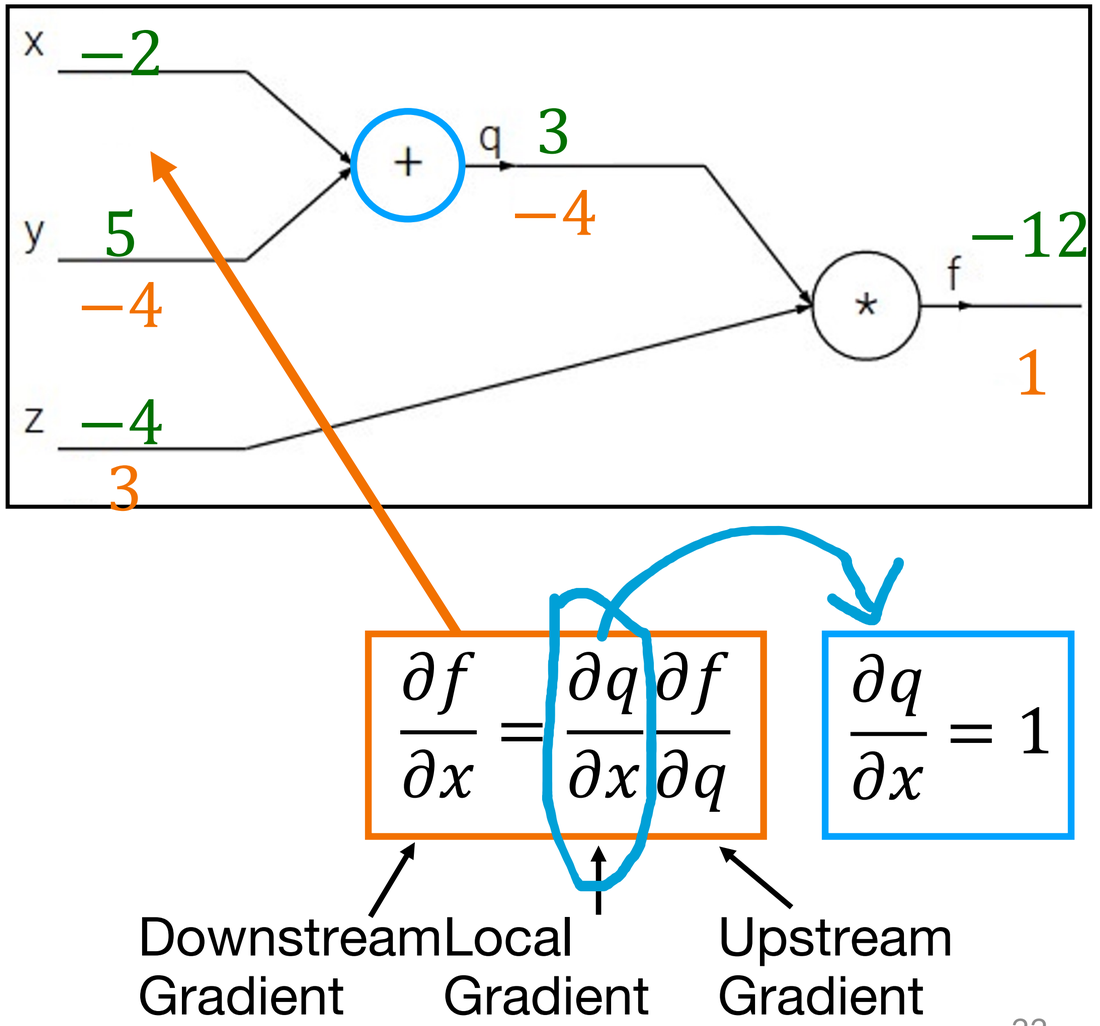
$$q = x + y \qquad f = q \cdot z$$

2. Backward pass: Compute derivatives

Want: $\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z}$



Backpropagation: Simple Example

$$f(x, y, z) = (x + y) \cdot z$$

e.g. $x = -2, y = 5, z = -4$

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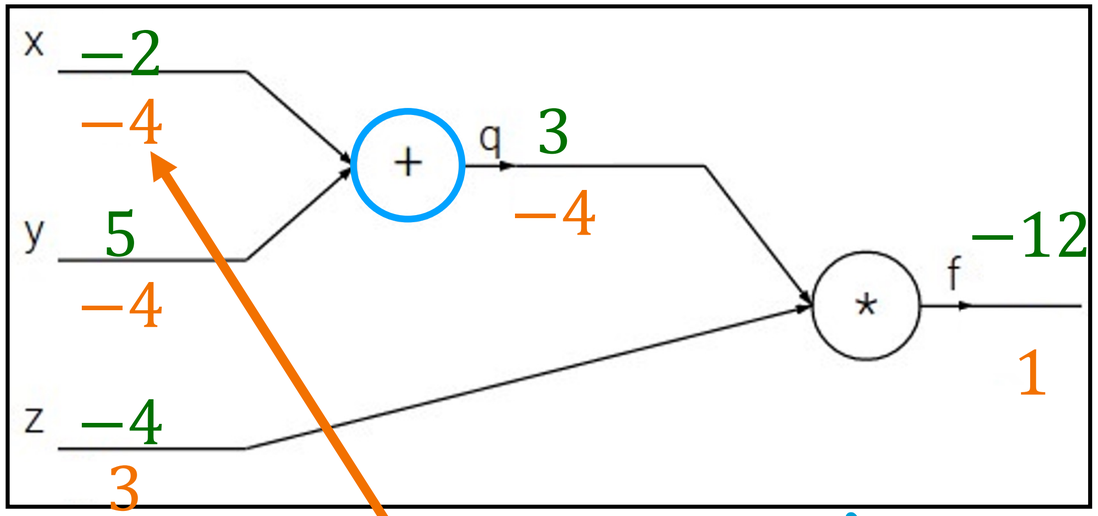
Want: $\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z}$



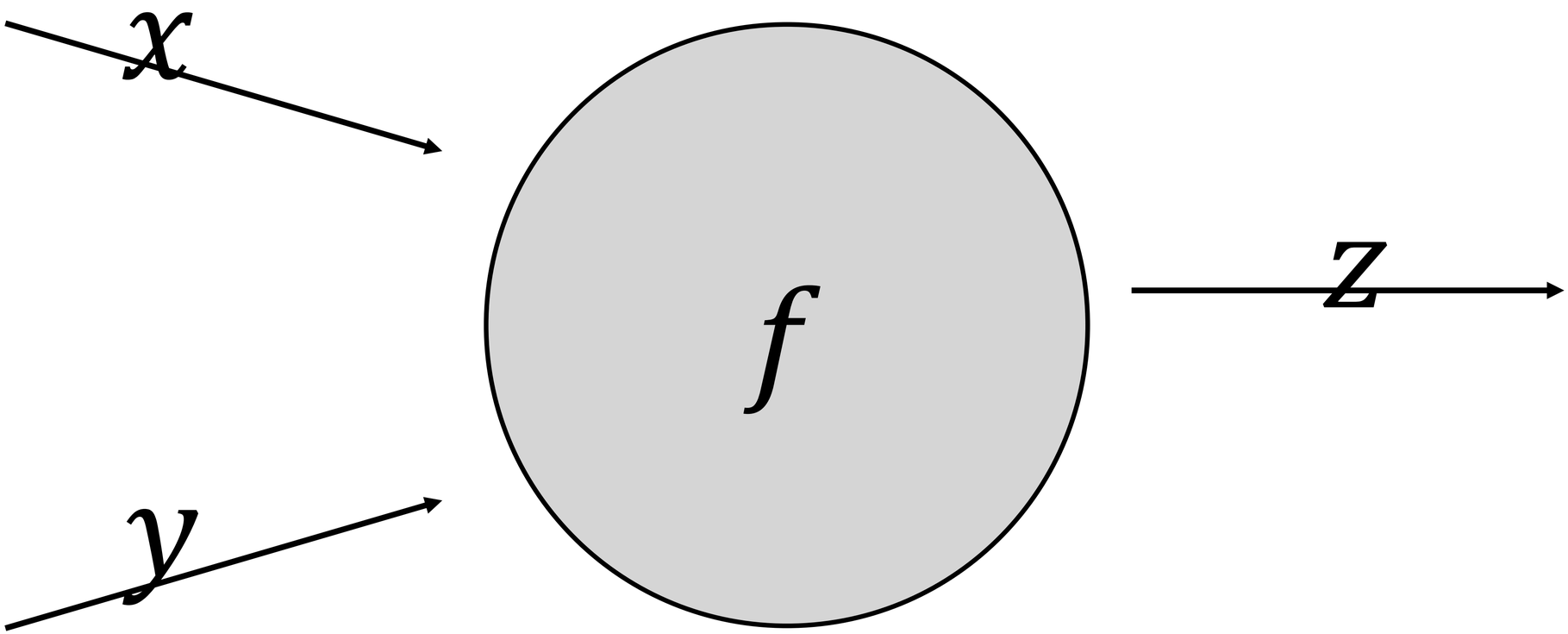
$$\frac{\partial f}{\partial x} = \frac{\partial q}{\partial x}\frac{\partial f}{\partial q}$$

$$\frac{\partial q}{\partial x} = 1$$

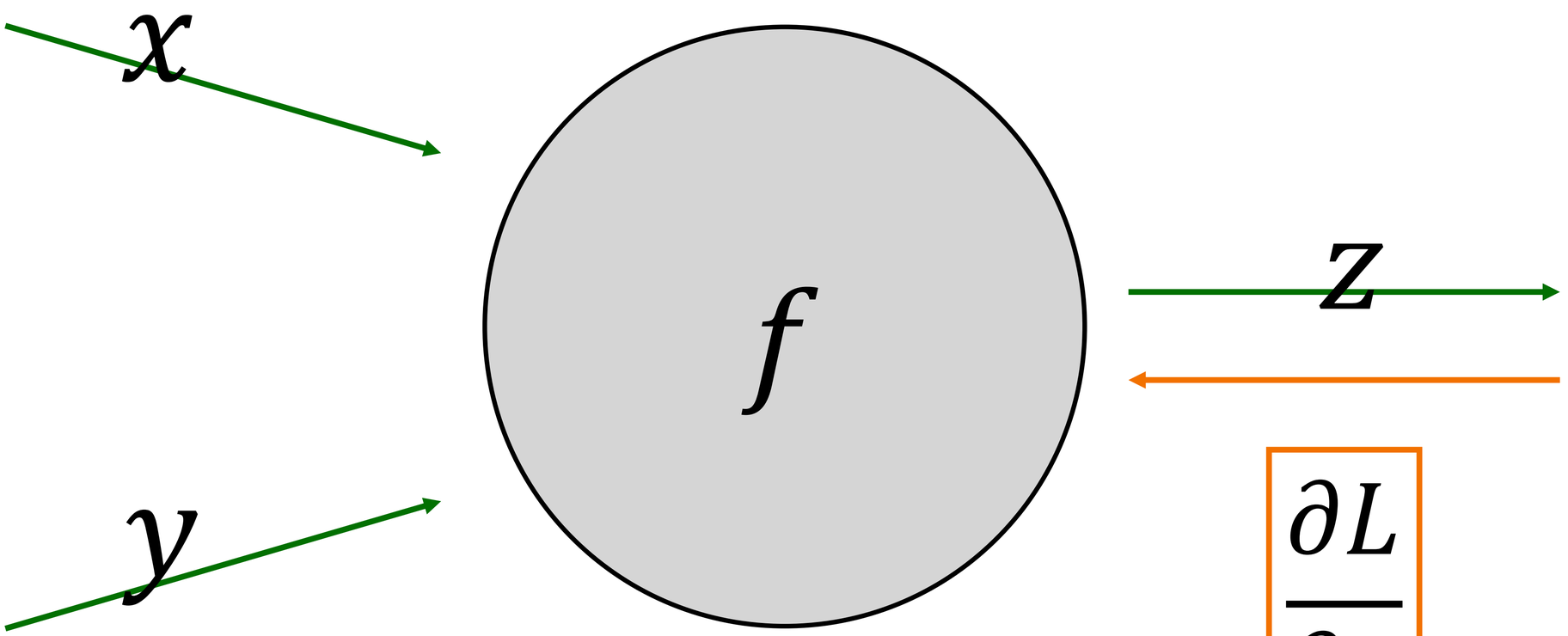
$$\frac{\partial f}{\partial q} = z = -4$$

Downstream Gradient | Local Gradient | Upstream Gradient

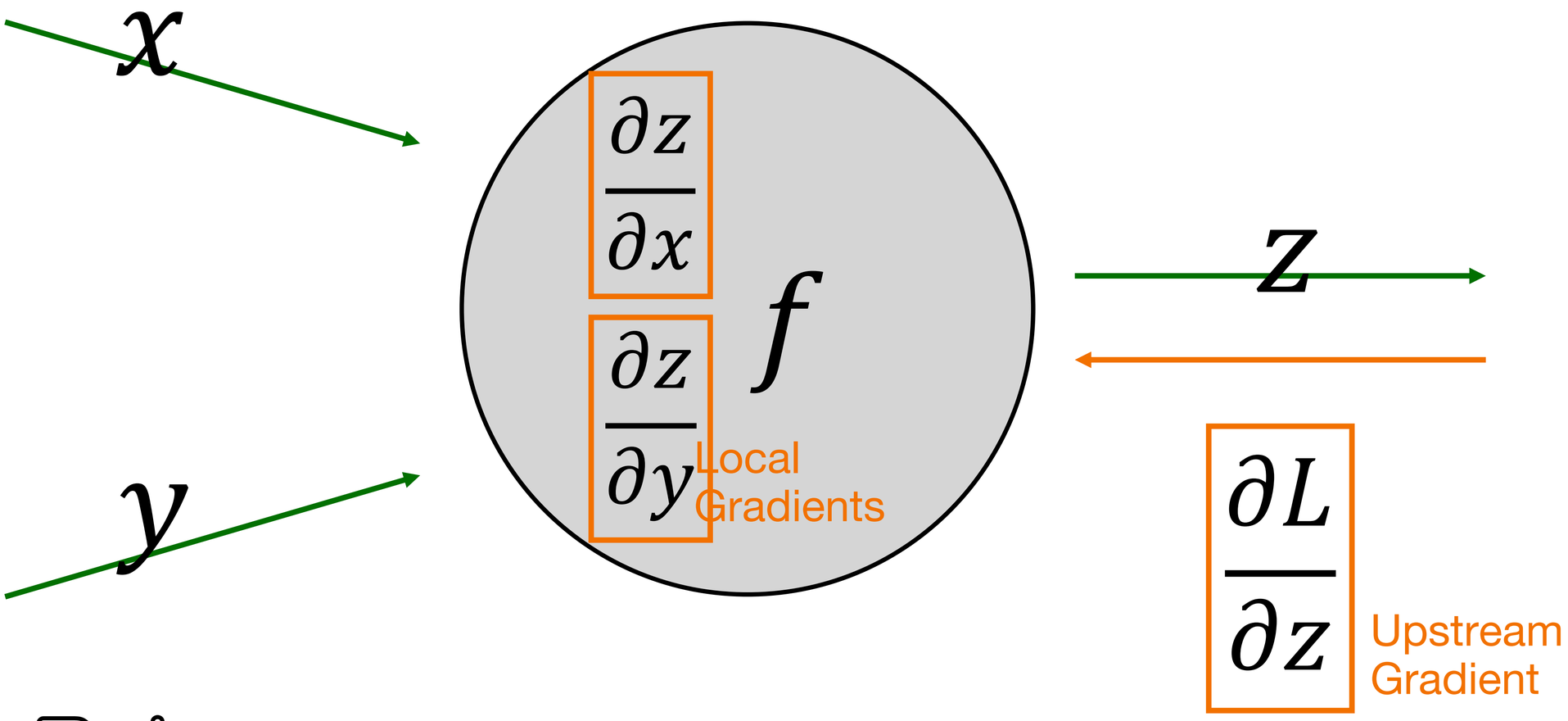
Local Properties of Backpropagation



Local Properties of Backpropagation

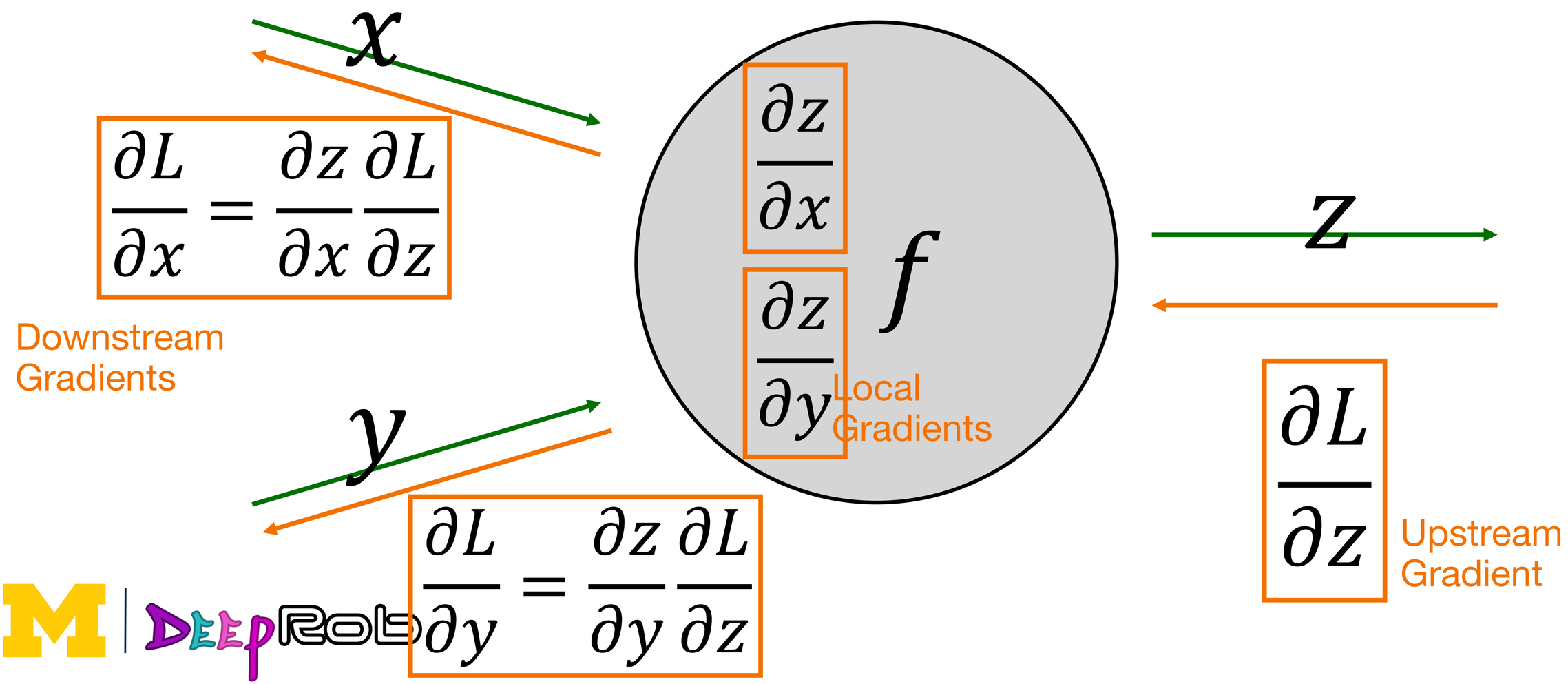


Local Properties of Backpropagation

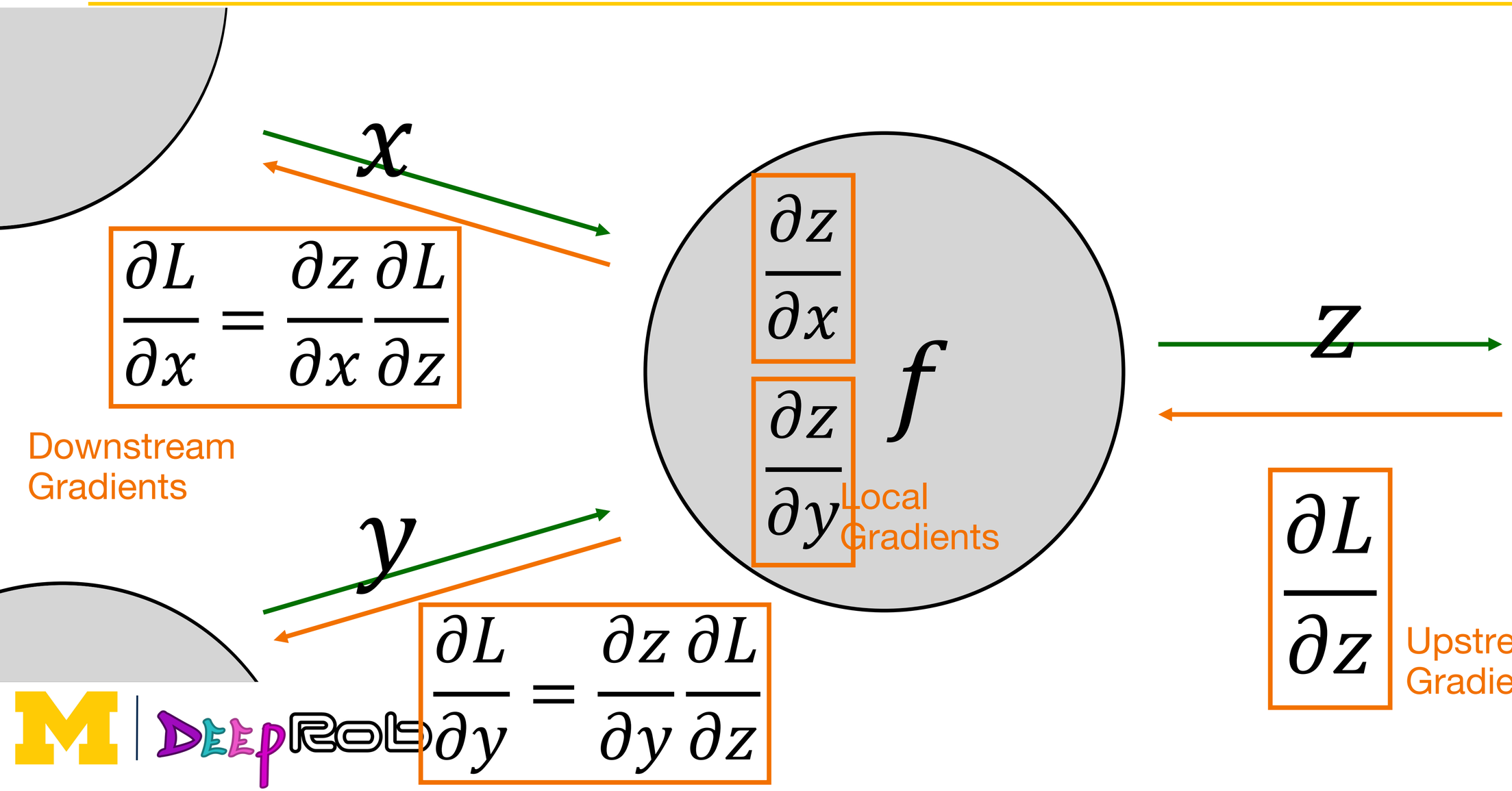


Local Properties of Backpropagation

"the chain rule"



Local Properties of Backpropagation



Another example

$$f(x, w) = \frac{1}{1 + e^{-(w_0 x_0 + w_1 x_1 + w2)}}$$

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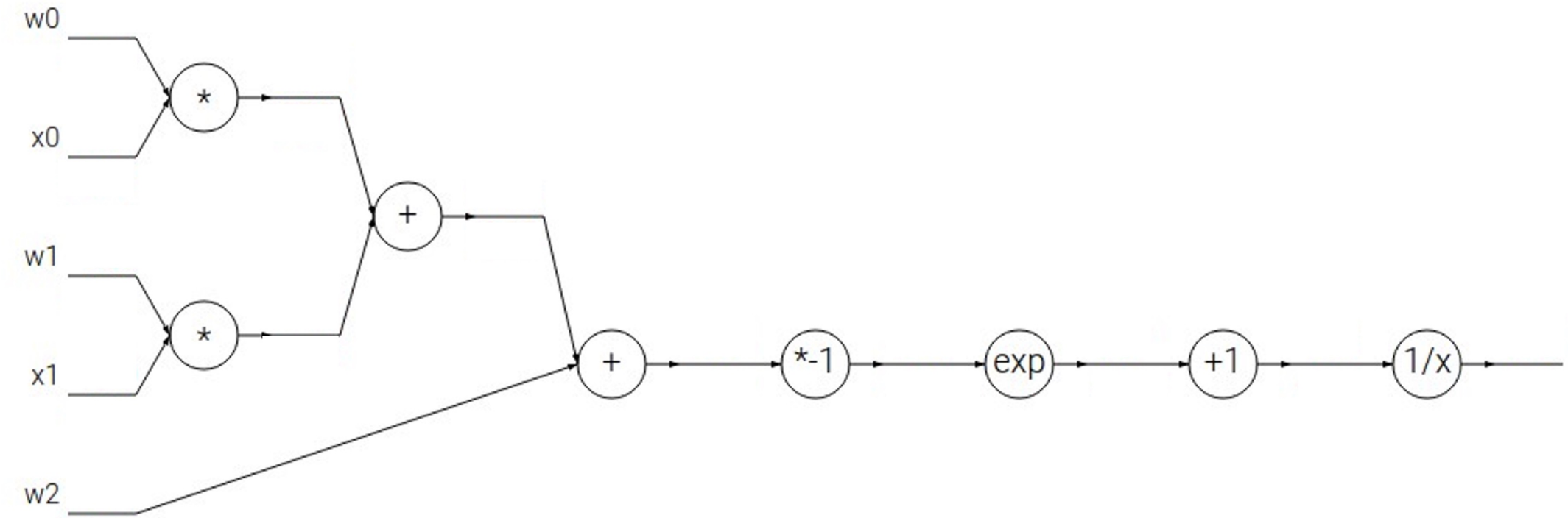
1. Forward pass: Compute outputs



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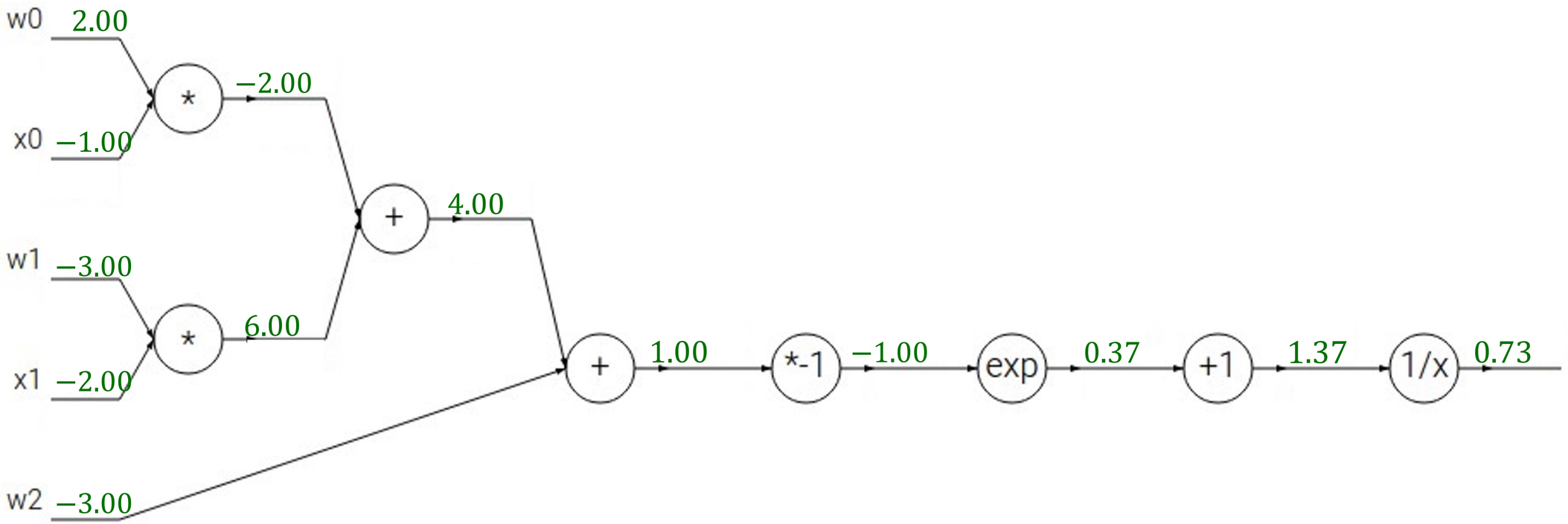
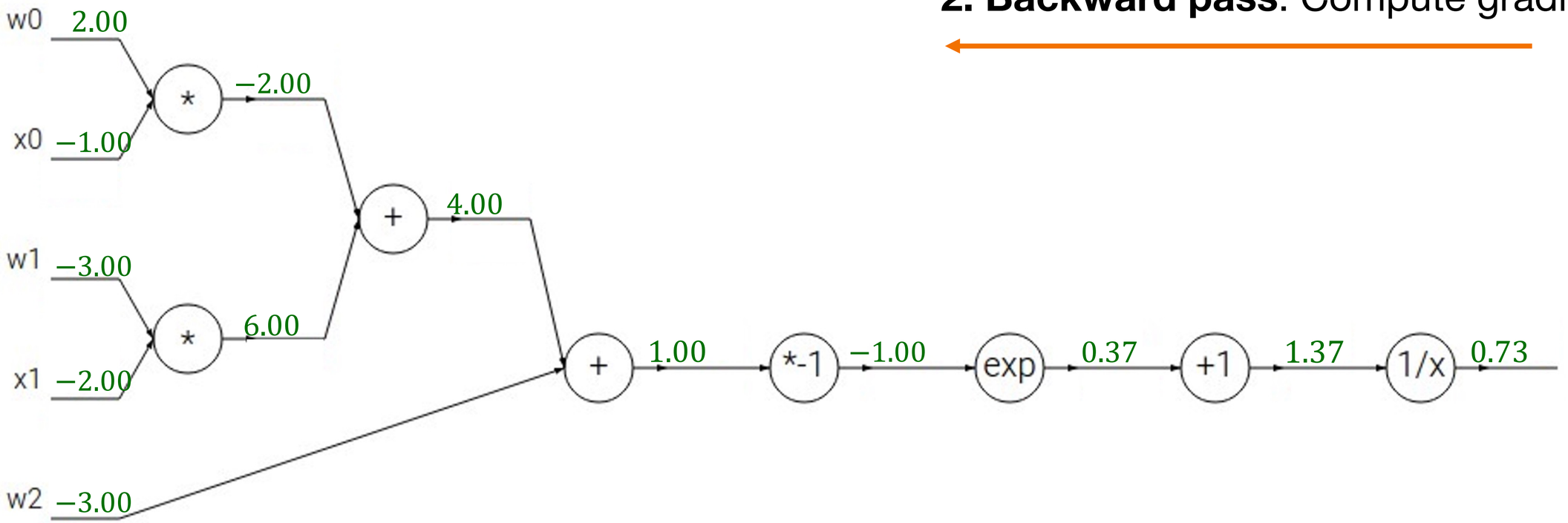


Another example

$$f(x,w) = \frac{1}{1 + e^{-(w_0 x_0 + w_1 x_1 + w2)}}$$

1. Forward pass: Compute outputs

2. Backward pass: Compute gradients



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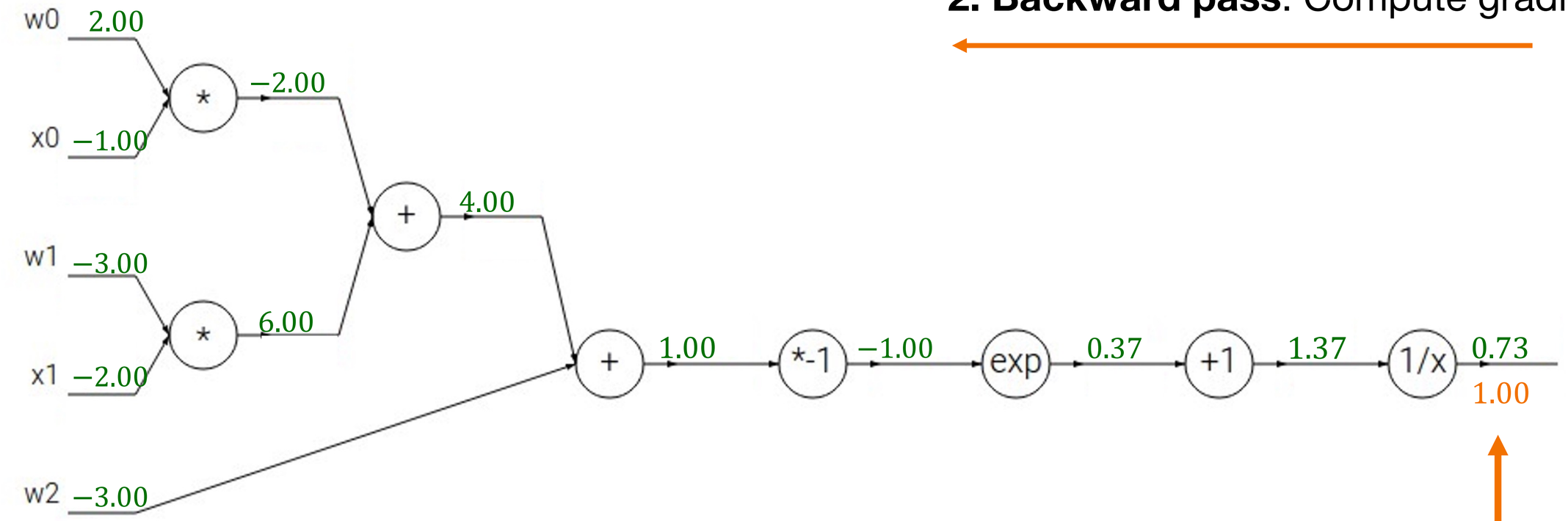


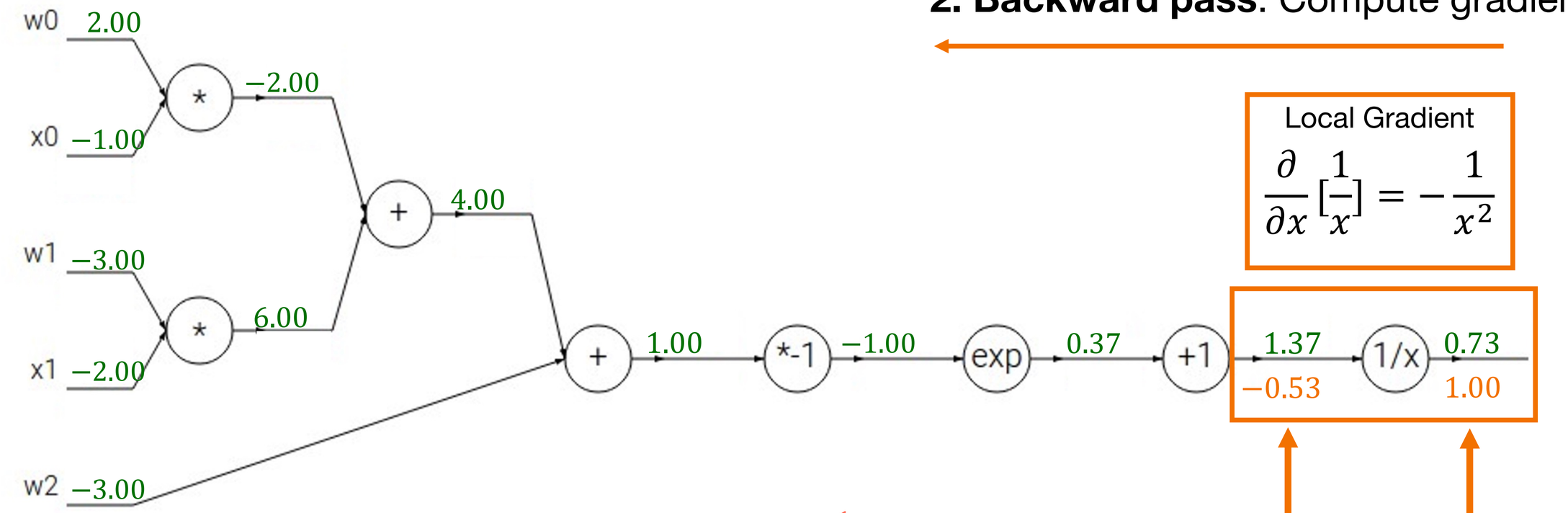
Base Case

Another example

$$f(x,w) = \frac{1}{1+e^{-(w_0x_0+w_1x_1+w2)}}$$

1. Forward pass: Compute outputs

2. Backward pass: Compute gradients



Local Gradient

$$\frac{\partial}{\partial x}\left[\frac{1}{x}\right] = -\frac{1}{x^2}$$

$$-\frac{1}{1.37^2} = -0.53$$

Downstream Gradient

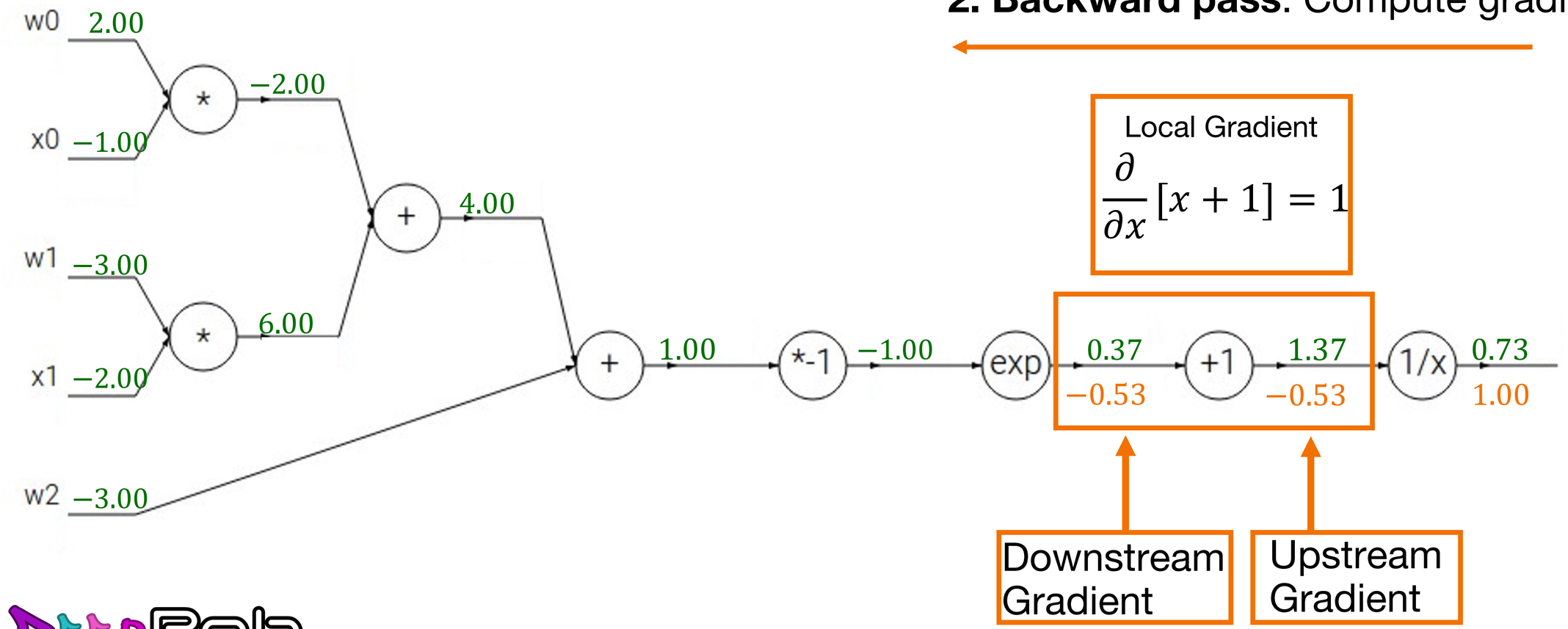
Upstream Gradient

Another example

$$f(x,w) = \frac{1}{1+e^{-(w_0x_0+w_1x_1+w2)}}$$

1. Forward pass: Compute outputs

2. Backward pass: Compute gradients



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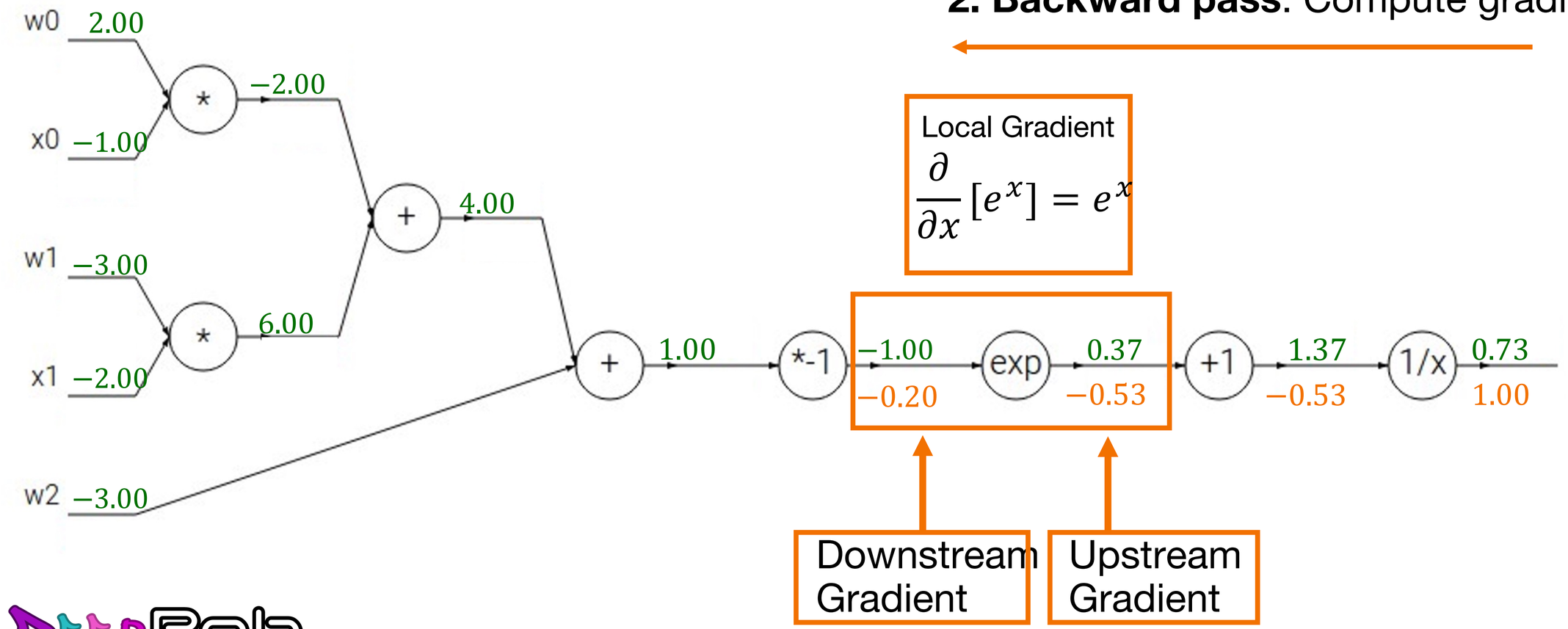

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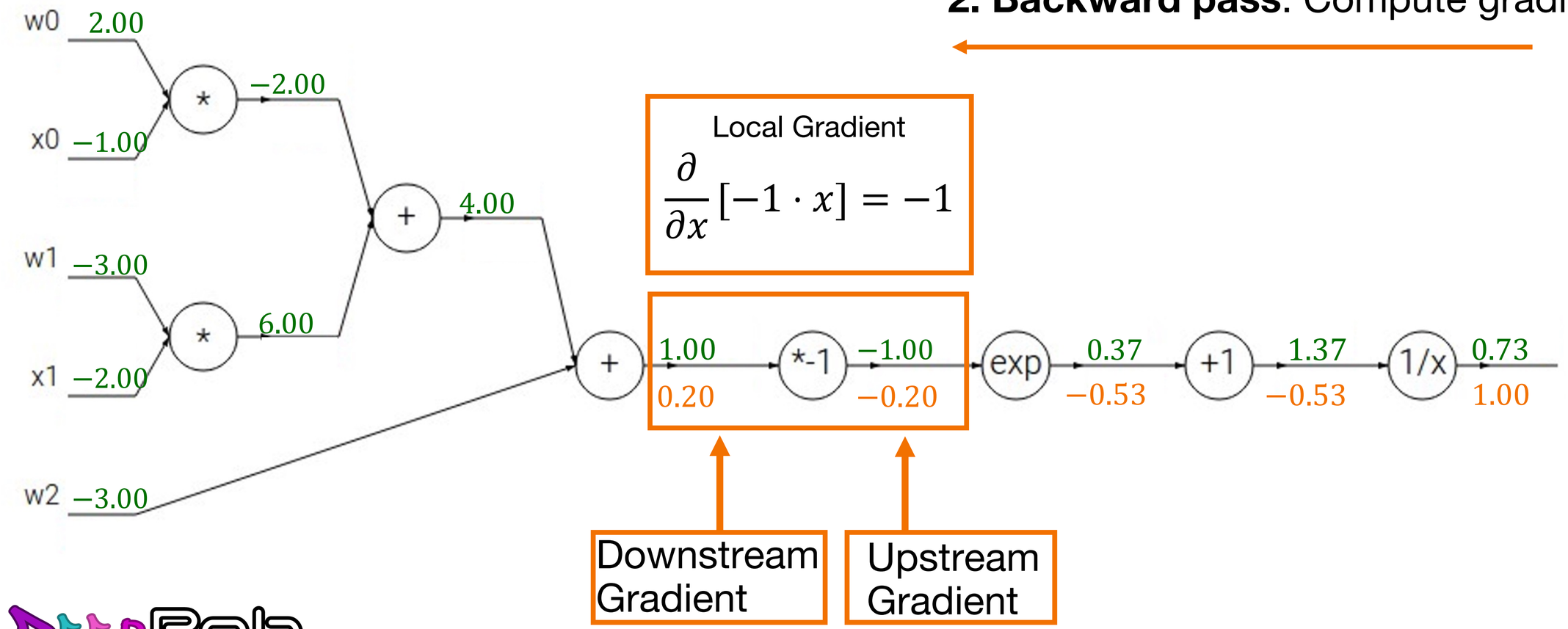

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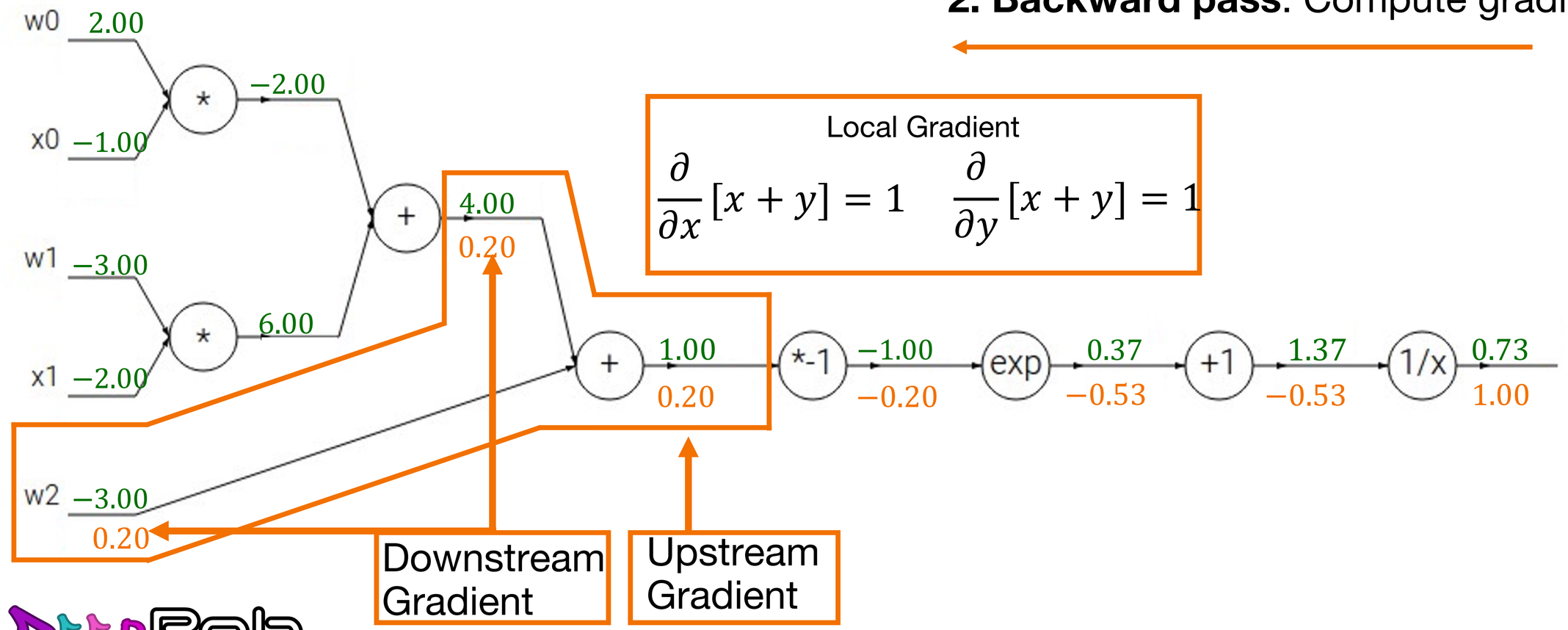
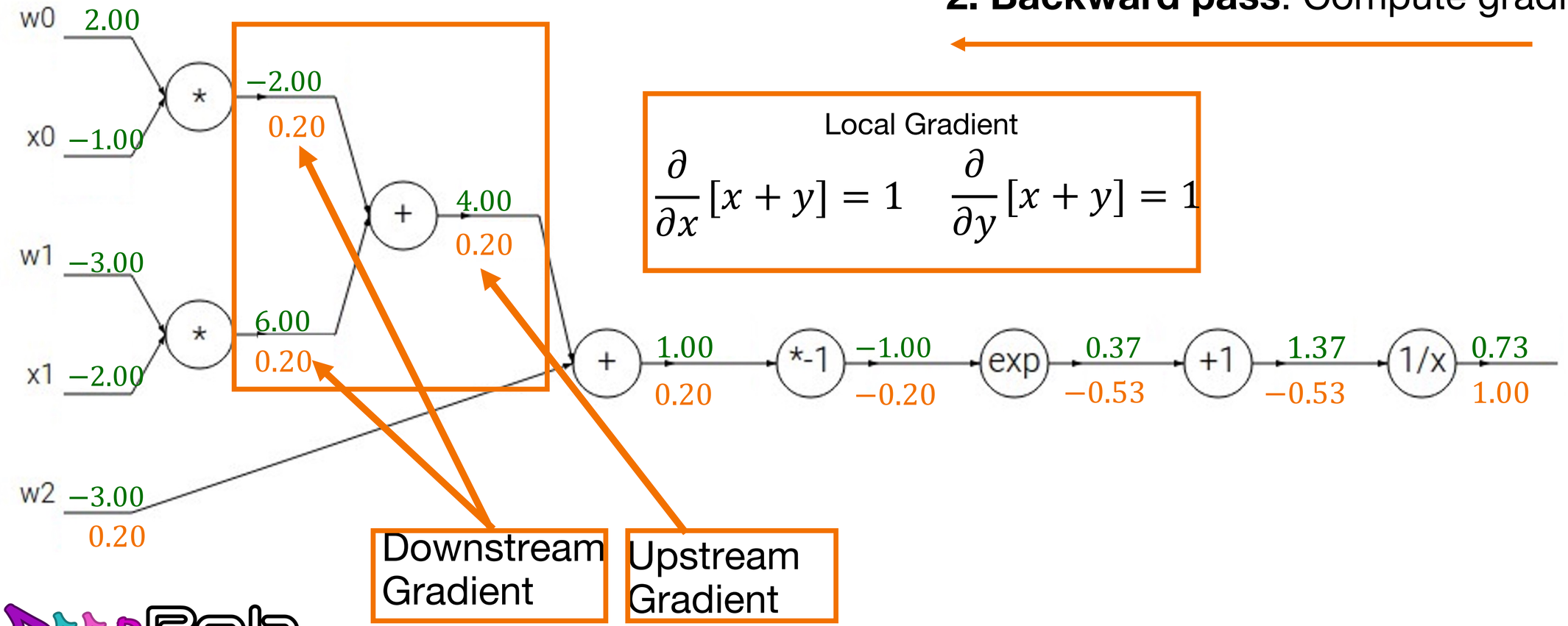


Another example

$$f(x,w) = \frac{1}{1+e^{-(w_0x_0+w_1x_1+w2)}}$$

1. Forward pass: Compute outputs

2. Backward pass: Compute gradients



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1. Forward pass: Compute outputs

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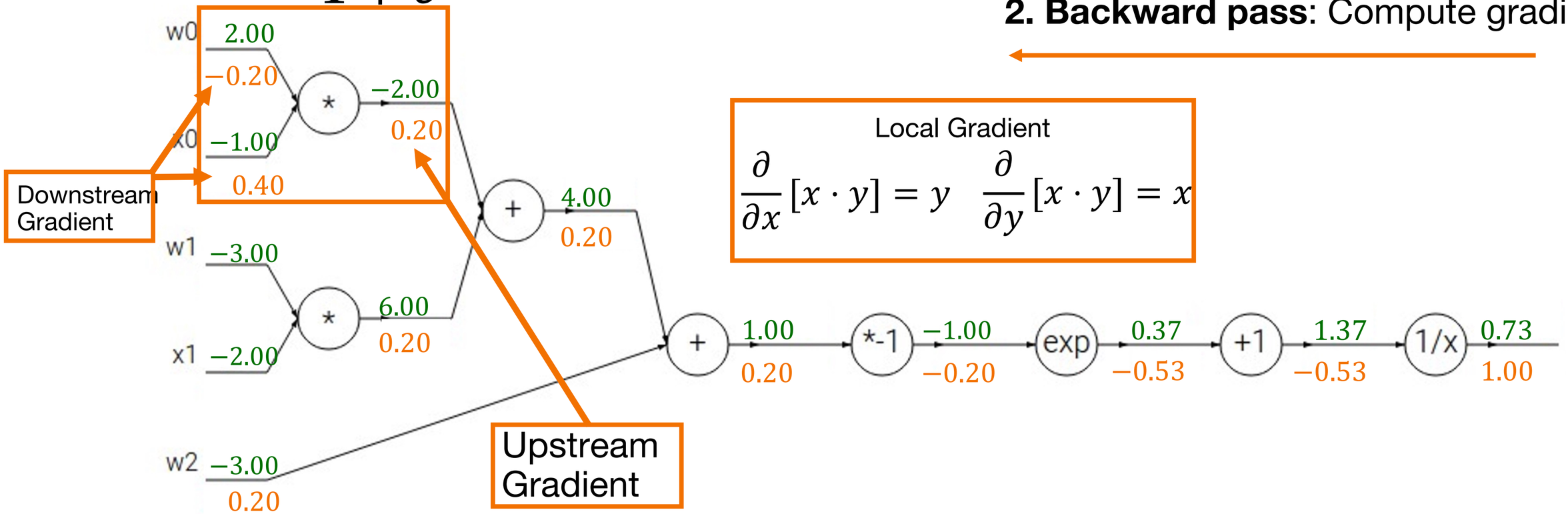


Local Gradient

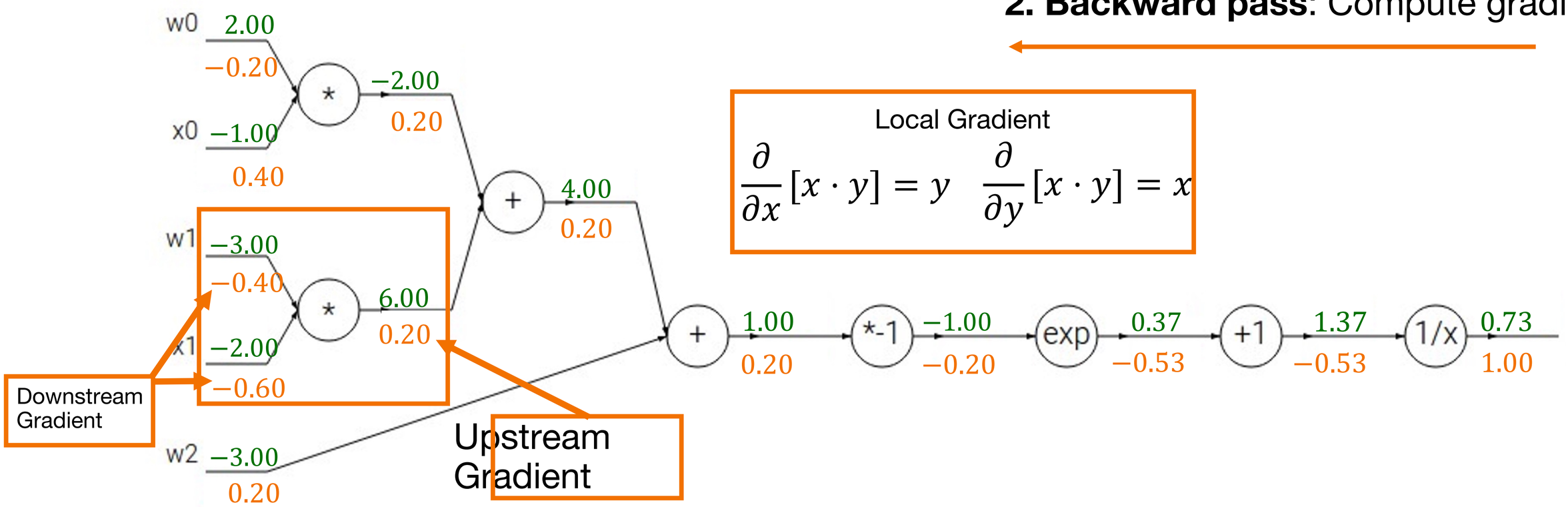
$$\frac{\partial}{\partial x}[x \cdot y] = y \quad \frac{\partial}{\partial y}[x \cdot y] = x$$

Another example

$$f(x,w) = \frac{1}{1+e^{-(w_0x_0+w_1x_1+w2)}}$$

1. Forward pass: Compute outputs

2. Backward pass: Compute gradients



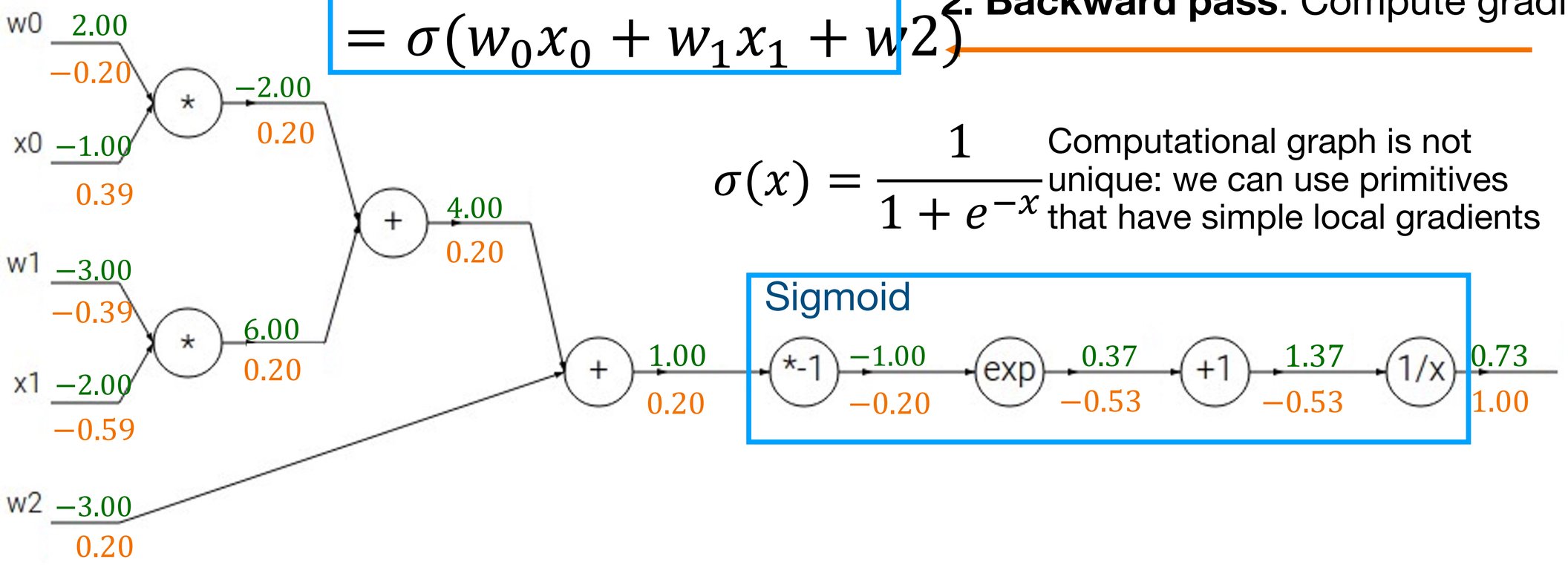
The Sigmoid

$$f(x,w) = \frac{1}{1+e^{-(w_0x_0+w_1x_1+w2)}}$$

$$= \sigma(w_0x_0 + w_1x_1 + w2)$$

1. Forward pass: Compute outputs

2. Backward pass: Compute gradients



$$\sigma(x) = \frac{1}{1+e^{-x}}$$

Computational graph is not unique: we can use primitives that have simple local gradients

The Sigmoid

$$f(x,w) = \frac{1}{1+e^{-(w_0x_0+w_1x_1+w2)}}$$

$$= \sigma(w_0x_0 + w_1x_1 + w2)$$

1. Forward pass: Compute outputs

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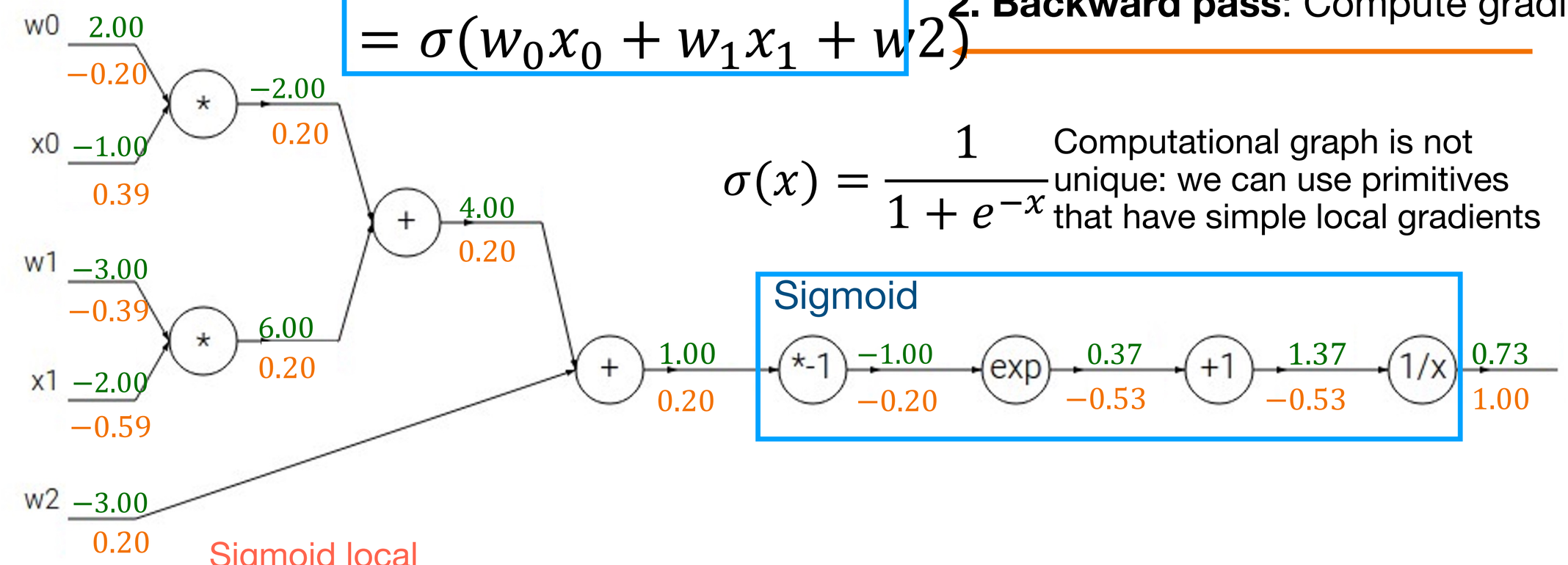


$$\sigma(x) = \frac{1}{1+e^{-x}}$$

Computational graph is not unique: we can use primitives that have simple local gradients

Sigmoid local gradient:

$$\frac{\partial}{\partial x}[\sigma(x)] = \frac{e^{-x}}{(1+e^{-x})^2} = \left(\frac{1+e^{-x}-1}{1+e^{-x}}\right)\left(\frac{1}{1+e^{-x}}\right) = (1-\sigma(x))\sigma(x)$$

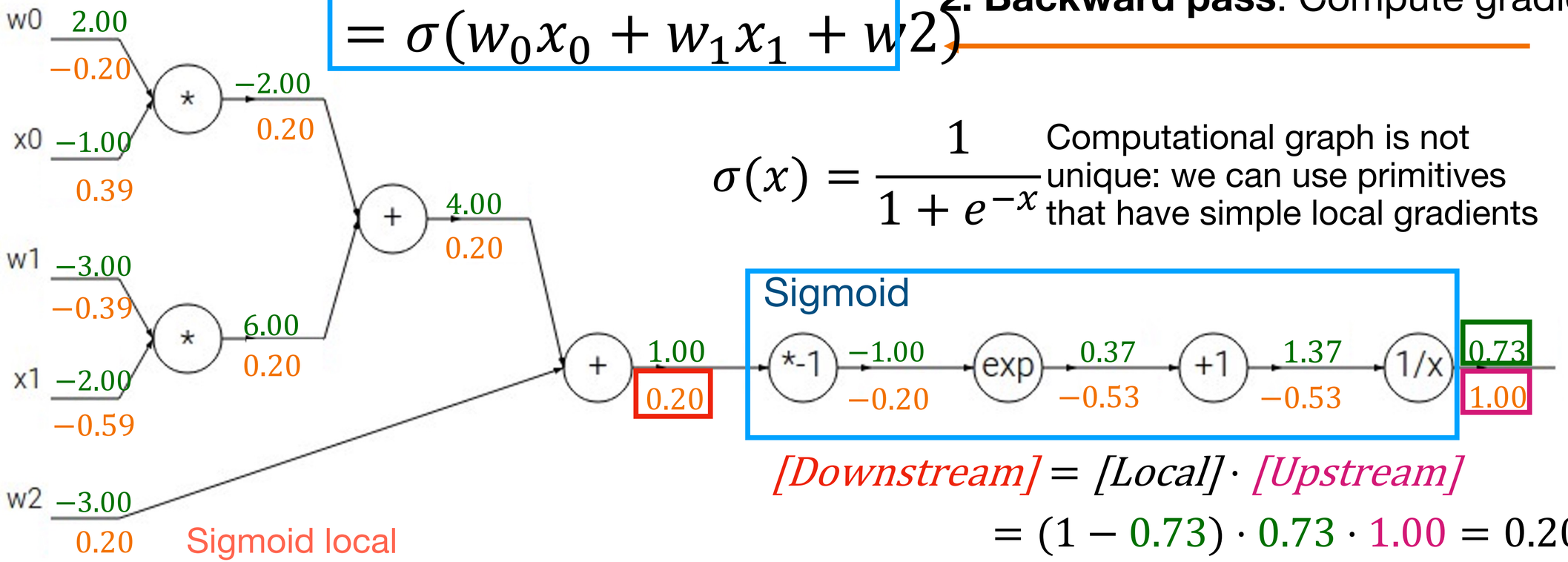
The Sigmoid

$$f(x,w) = \frac{1}{1+e^{-(w_0x_0+w_1x_1+w2)}}$$

$$= \sigma(w_0x_0 + w_1x_1 + w2)$$

1. Forward pass: Compute outputs

2. Backward pass: Compute gradients



$$\sigma(x) = \frac{1}{1+e^{-x}}$$

Computational graph is not unique: we can use primitives that have simple local gradients

$$[Downstream] = [Local] \cdot [Upstream]$$

$$= (1 - 0.73) \cdot 0.73 \cdot 1.00 = 0.20$$

Sigmoid local gradient:

$$\frac{\partial}{\partial x}[\sigma(x)] = \frac{e^{-x}}{(1+e^{-x})^2} = \left(\frac{1+e^{-x}-1}{1+e^{-x}}\right)\left(\frac{1}{1+e^{-x}}\right) = (1-\sigma(x))\sigma(x)$$

Other Common Functions

$$f(x) = e^x \longrightarrow \frac{df}{dx} = e^x$$

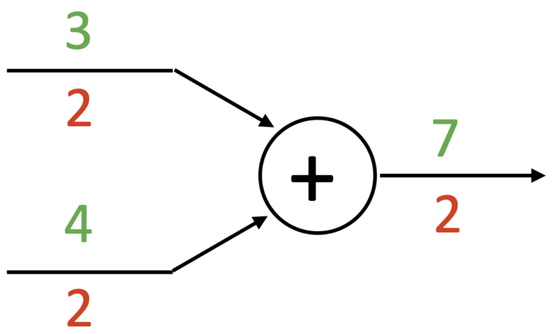
$$f_a(x) = ax \longrightarrow \frac{df}{dx} = a$$

$$f(x) = \frac{1}{x} \longrightarrow \frac{df}{dx} = -1/x^2$$

$$f_c(x) = c + x \longrightarrow \frac{df}{dx} = 1$$

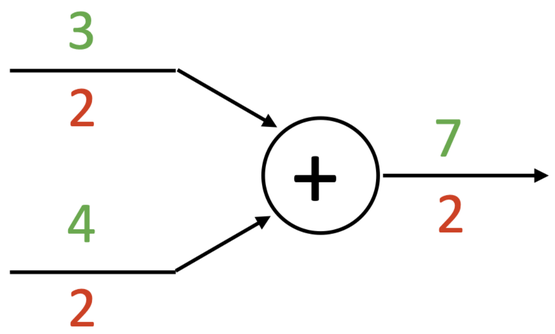
Patterns in Gradient Flow

add gate: gradient distributor

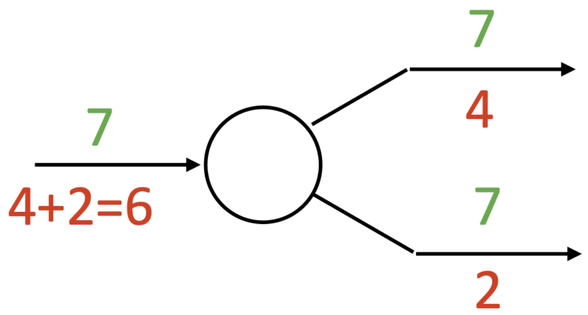


Patterns in Gradient Flow

add gate: gradient distributor

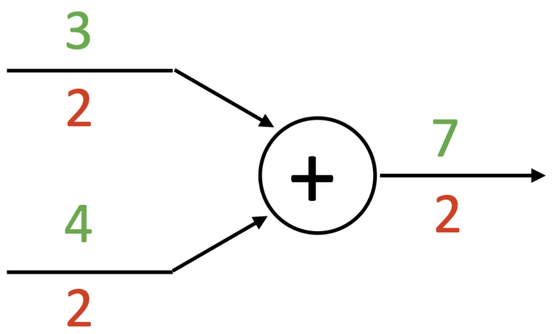


copy gate: gradient adder

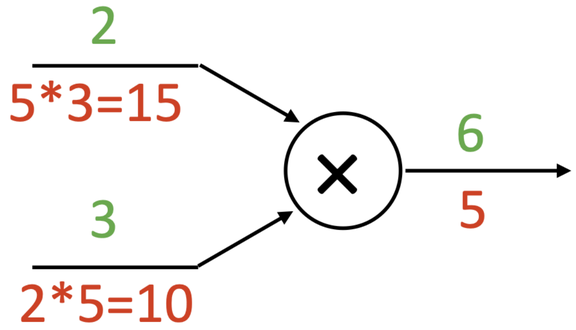


Patterns in Gradient Flow

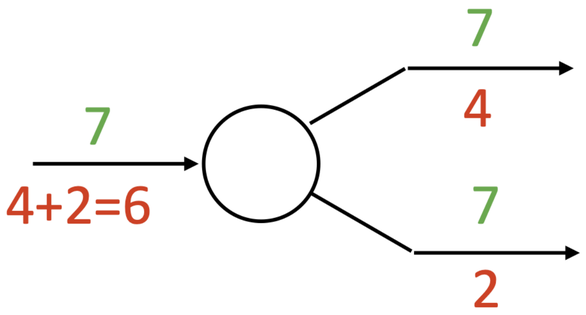
add gate: gradient distributor



mul gate: “swap multiplier”

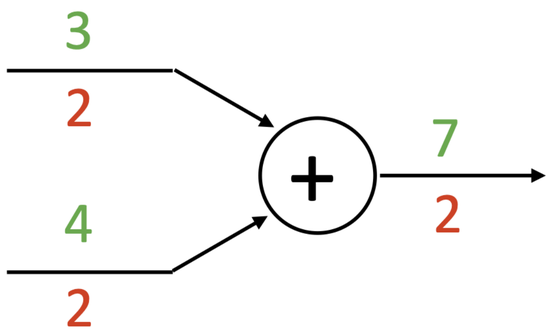


copy gate: gradient adder



Patterns in Gradient Flow

add gate: gradient distributor



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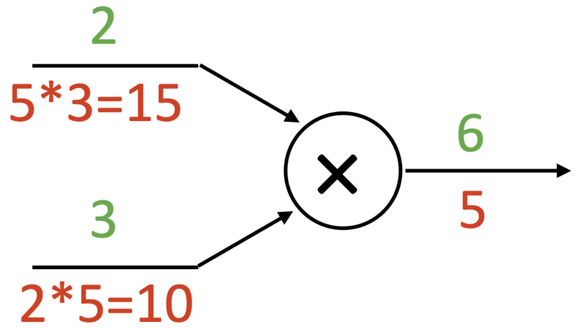
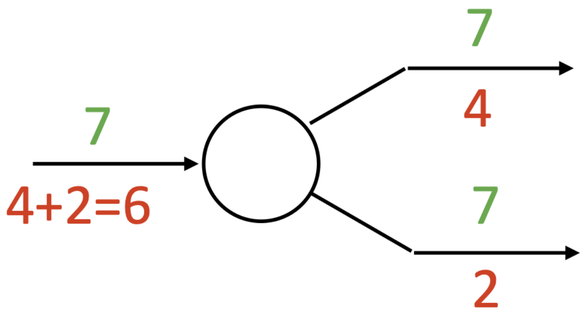
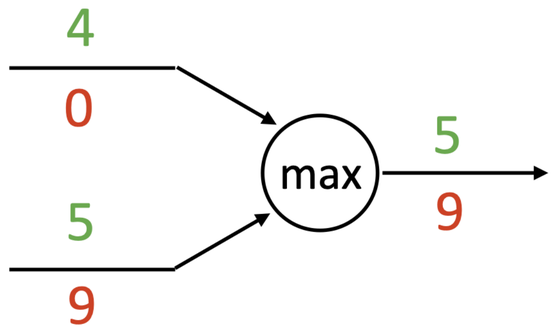


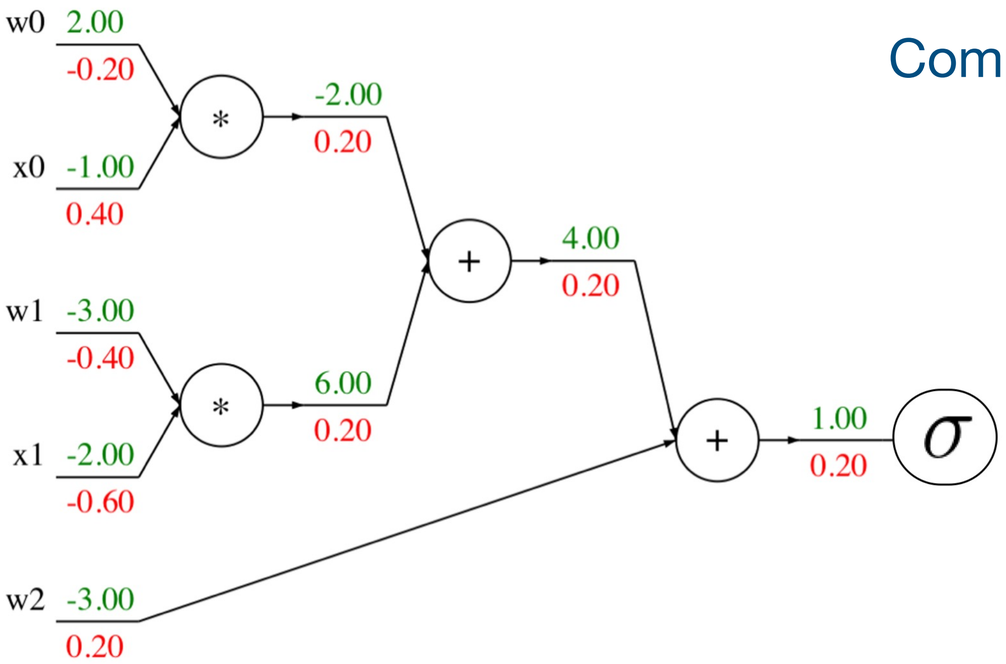
copy gate: gradient adder



max gate: gradient router



Backprop Implementation: “Flat” gradient code

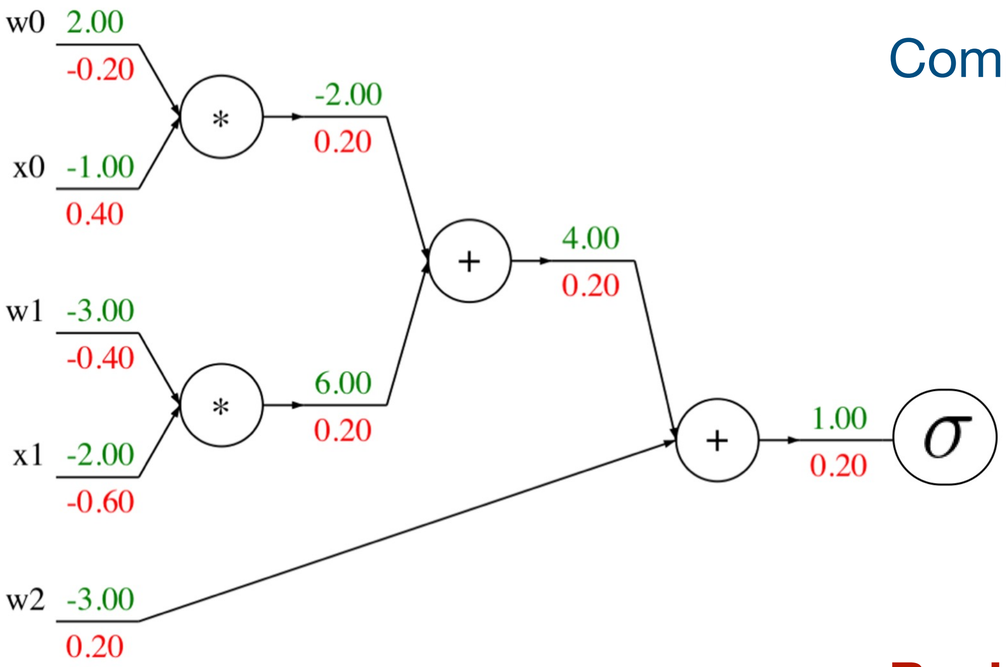


Forward pass:

Compute outputs

```
def f(w0, x0, w1, x1, w2):
  s0 = w0 * x0
  s1 = w1 * x1
  s2 = s0 + s1
  s3 = s2 + w2
  L = sigmoid(s3)
```

Backprop Implementation: “Flat” gradient code



Forward pass:

Compute outputs

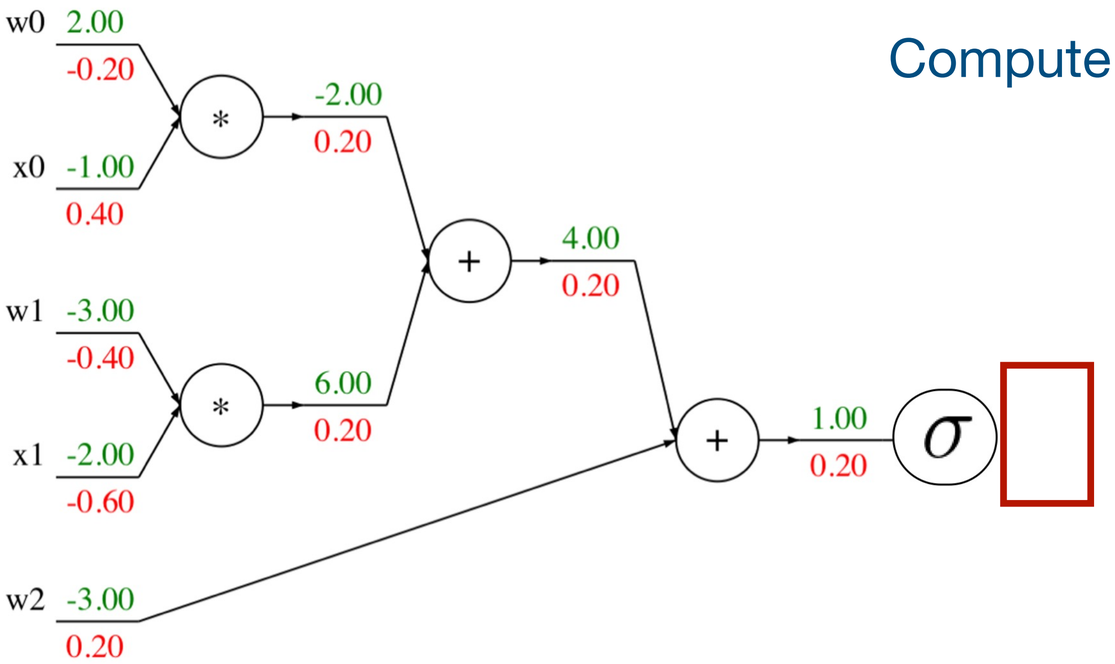
```
def f(w0, x0, w1, x1, w2):
  s0 = w0 * x0
  s1 = w1 * x1
  s2 = s0 + s1
  s3 = s2 + w2
  L = sigmoid(s3)
```

Backward pass:

Compute gradients

```
grad_L = 1.0
grad_s3 = grad_L * (1 - L) * L
grad_w2 = grad_s3
grad_s2 = grad_s3
grad_s0 = grad_s2
grad_s1 = grad_s2
grad_w1 = grad_s1 * x1
grad_x1 = grad_s1 * w1
grad_w0 = grad_s0 * x0
grad_x0 = grad_s0 * w0
```

Backprop Implementation: “Flat” gradient code



Forward pass:

Compute outputs

```
def f(w0, x0, w1, x1, w2):
  s0 = w0 * x0
  s1 = w1 * x1
  s2 = s0 + s1
  s3 = s2 + w2
  L = sigmoid(s3)
```

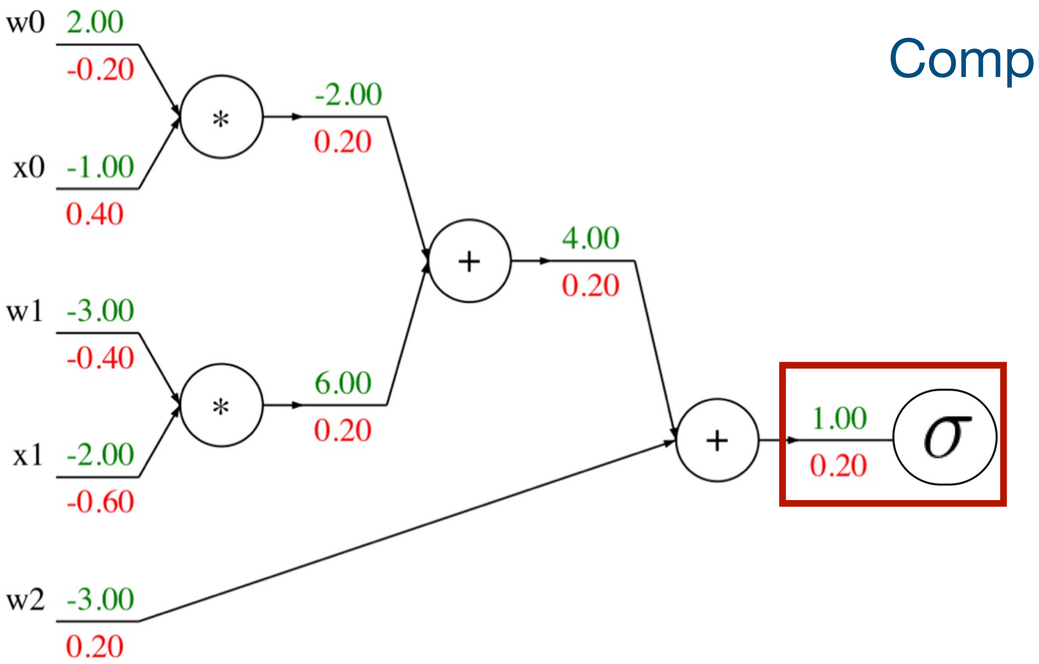
Base case

```
grad_L = 1.0
grad_s3 = grad_L * (1 - L) * L
grad_w2 = grad_s3
grad_s2 = grad_s3
grad_s0 = grad_s2
grad_s1 = grad_s2
grad_w1 = grad_s1 * x1
grad_x1 = grad_s1 * w1
grad_w0 = grad_s0 * x0
grad_x0 = grad_s0 * w0
```

Backward pass:

Compute gradients

Backprop Implementation: “Flat” gradient code



Forward pass:

Compute outputs

```
def f(w0, x0, w1, x1, w2):
  s0 = w0 * x0
  s1 = w1 * x1
  s2 = s0 + s1
  s3 = s2 + w2
  L = sigmoid(s3)
```

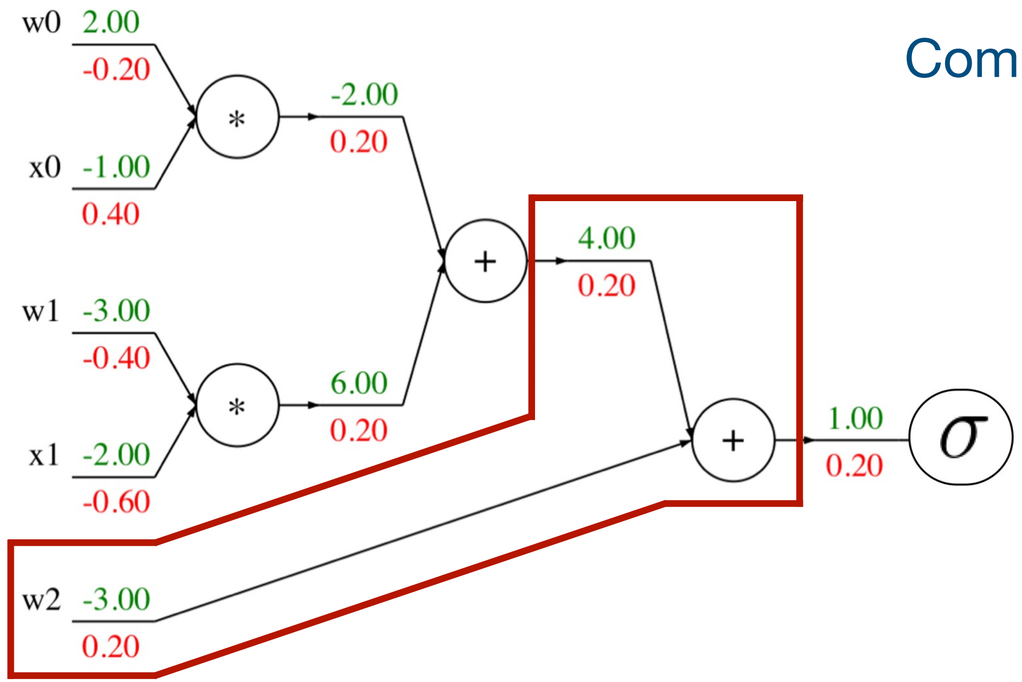
Sigmoid

```
grad_L = 1.0
grad_s3 = grad_L * (1 - L) * L
grad_w2 = grad_s3
grad_s2 = grad_s3
grad_s0 = grad_s2
grad_s1 = grad_s2
grad_w1 = grad_s1 * x1
grad_x1 = grad_s1 * w1
grad_w0 = grad_s0 * x0
grad_x0 = grad_s0 * w0
```

Backward pass:

Compute gradients

Backprop Implementation: “Flat” gradient code



Forward pass:

Compute outputs

```
def f(w0, x0, w1, x1, w2):
  s0 = w0 * x0
  s1 = w1 * x1
  s2 = s0 + s1
  s3 = s2 + w2
  L = sigmoid(s3)
```

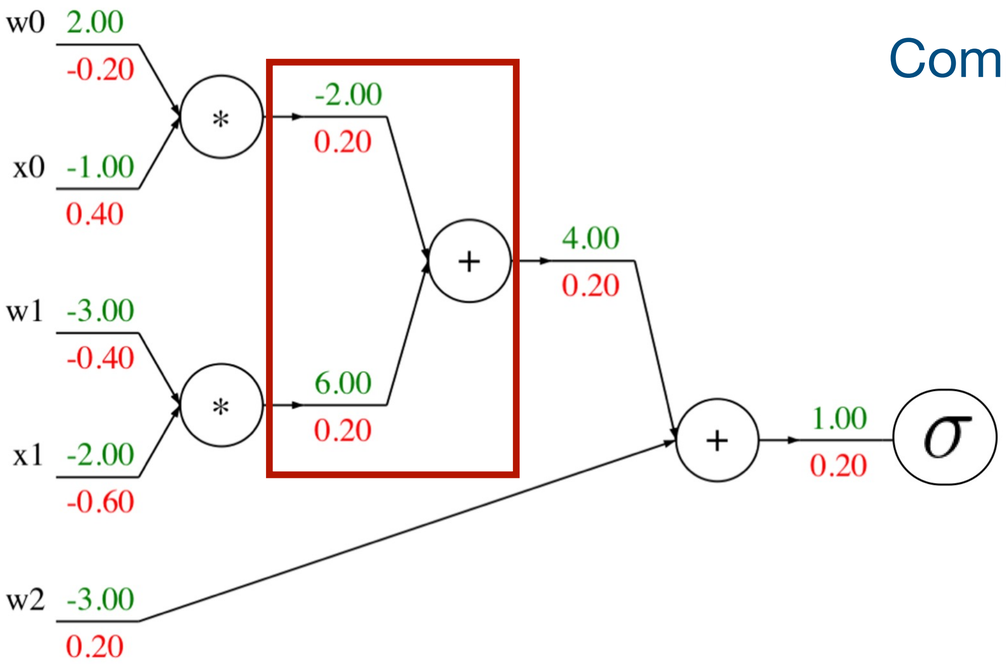
Add

Backward pass:

Compute gradients

```
grad_L = 1.0
grad_s3 = grad_L * (1 - L) * L
grad_w2 = grad_s3
grad_s2 = grad_s3
grad_s0 = grad_s2
grad_s1 = grad_s2
grad_w1 = grad_s1 * x1
grad_x1 = grad_s1 * w1
grad_w0 = grad_s0 * x0
grad_x0 = grad_s0 * w0
```

Backprop Implementation: “Flat” gradient code



Forward pass:

Compute outputs

```
def f(w0, x0, w1, x1, w2):
  s0 = w0 * x0
  s1 = w1 * x1
  s2 = s0 + s1
  s3 = s2 + w2
  L = sigmoid(s3)
```

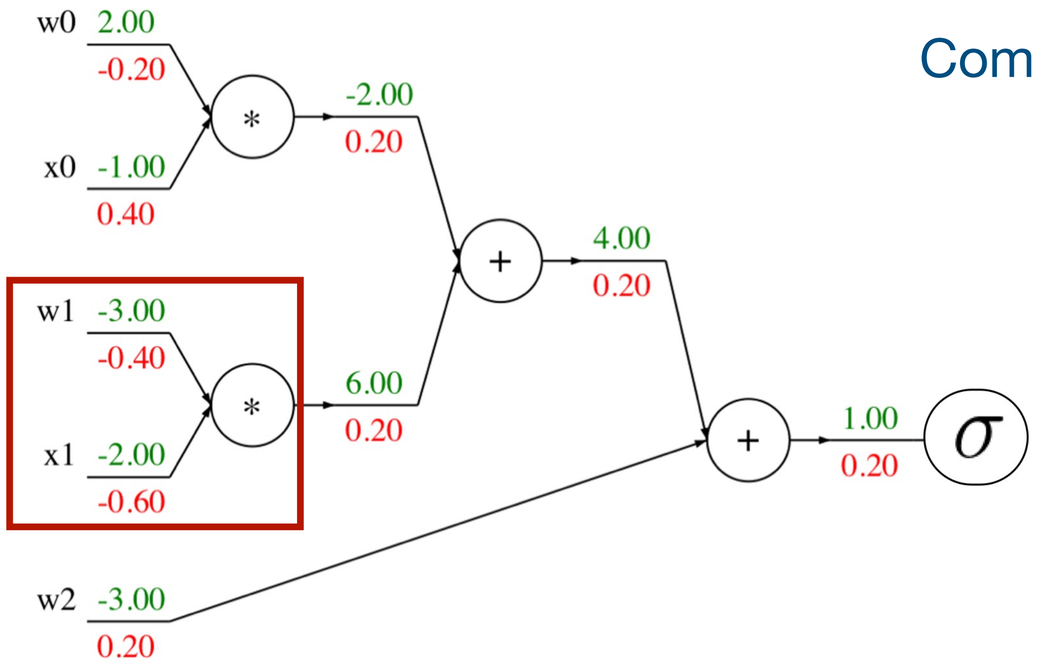
Add

```
grad_L = 1.0
grad_s3 = grad_L * (1 - L) * L
grad_w2 = grad_s3
grad_s2 = grad_s3
grad_s0 = grad_s2
grad_s1 = grad_s2
grad_w1 = grad_s1 * x1
grad_x1 = grad_s1 * w1
grad_w0 = grad_s0 * x0
grad_x0 = grad_s0 * w0
```

Backward pass:

Compute gradients

Backprop Implementation: “Flat” gradient code



Forward pass:

Compute outputs

```
def f(w0, x0, w1, x1, w2):
  s0 = w0 * x0
  s1 = w1 * x1
  s2 = s0 + s1
  s3 = s2 + w2
  L = sigmoid(s3)
```

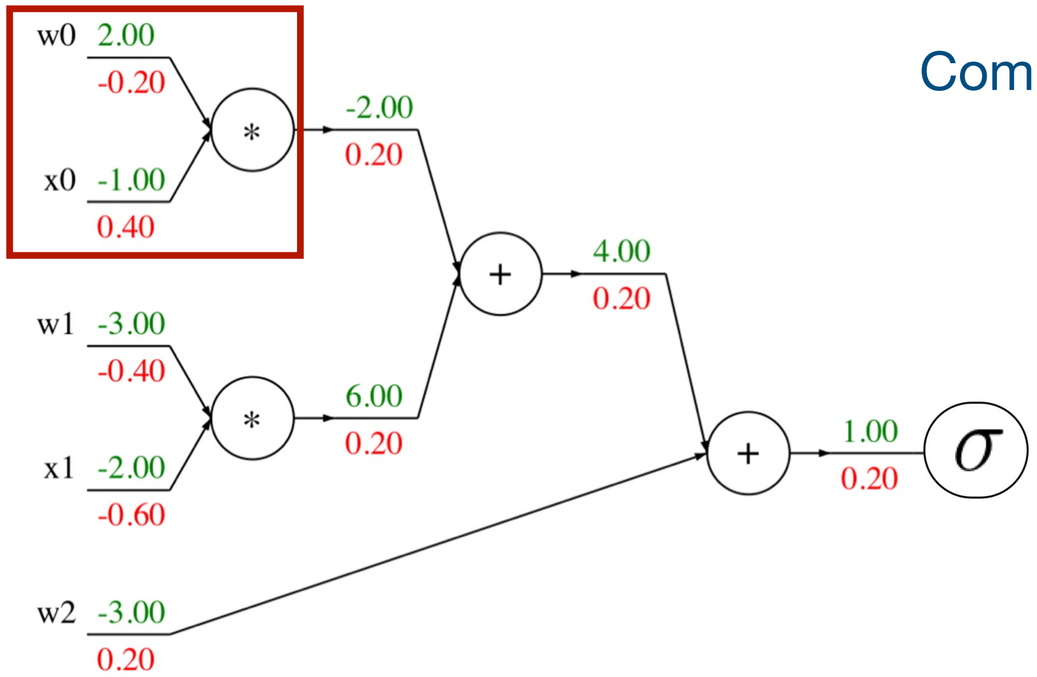
Multiply

```
grad_L = 1.0
grad_s3 = grad_L * (1 - L) * L
grad_w2 = grad_s3
grad_s2 = grad_s3
grad_s0 = grad_s2
grad_s1 = grad_s2
grad_w1 = grad_s1 * x1
grad_x1 = grad_s1 * w1
grad_w0 = grad_s0 * x0
grad_x0 = grad_s0 * w0
```

Backward pass:

Compute gradients

Backprop Implementation: “Flat” gradient code



Forward pass:

Compute outputs

```
def f(w0, x0, w1, x1, w2):
  s0 = w0 * x0
  s1 = w1 * x1
  s2 = s0 + s1
  s3 = s2 + w2
  L = sigmoid(s3)
```

```
grad_L = 1.0
grad_s3 = grad_L * (1 - L) * L
grad_w2 = grad_s3
grad_s2 = grad_s3
grad_s0 = grad_s2
grad_s1 = grad_s2
grad_w1 = grad_s1 * x1
grad_x1 = grad_s1 * w1
grad_w0 = grad_s0 * x0
grad_x0 = grad_s0 * w0
```

Multiply

Backward pass:

Compute gradients

“Flat” Backprop: Do this for Project 1 & 2

Forward pass:

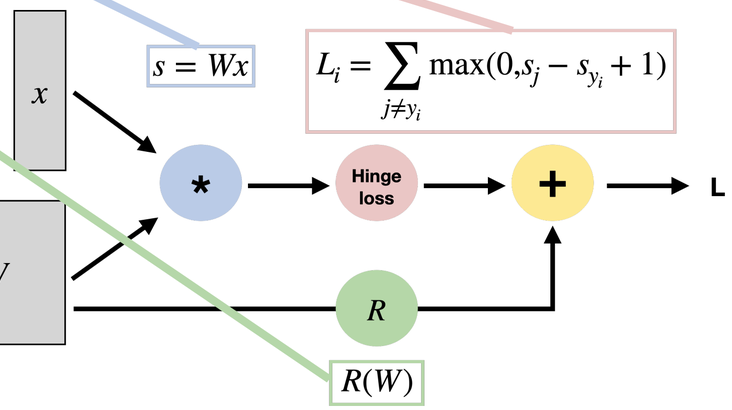
Compute outputs

```
##############################################################################
# TODO:                                                                      #
# Implement a vectorized version of the structured SVM loss, storing the    #
# result in loss.                                                            #
##############################################################################
# Replace "pass" statement with your code
num_classes = W.shape[1]
num_train = X.shape[0]
score = # ...
correct_class_score = # ...
margin = # ...
data_loss = # ...
reg_loss = # ...
loss += data_loss + reg_loss
##############################################################################
#                             END OF YOUR CODE                               #
##############################################################################
```

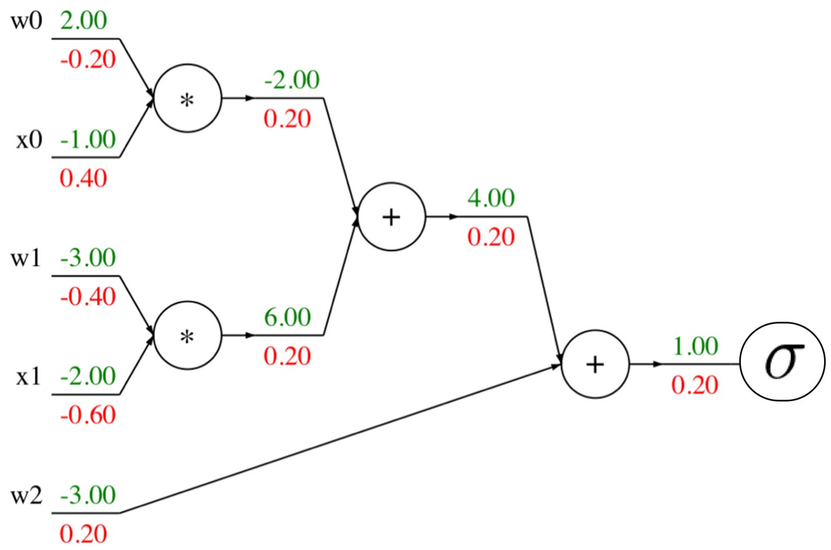
Backward pass:

Compute gradients

```
##############################################################################
# TODO:                                                                      #
# Implement a vectorized version of the gradient for the structured SVM     #
# loss, storing the result in dW.                                            #
#                                                                            #
# Hint: Instead of computing the gradient from scratch, it may be easier     #
# to reuse some of the intermediate values that you used to compute the      #
# loss.                                                                      #
##############################################################################
# Replace "pass" statement with your code
dmargins = # ...
dscores = # ...
dW = # ...
##############################################################################
#                             END OF YOUR CODE                               #
##############################################################################
```



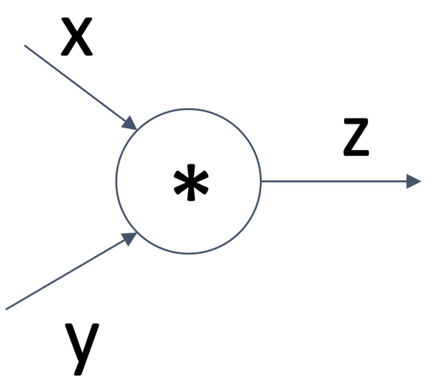
Backprop Implementation: Modular API



Graph (or Net) object *(rough pseudo code)*

```
class ComputationalGraph(object):
    #...
    def forward(inputs):
        # 1. [pass inputs to input gates...]
        # 2. forward the computational graph:
        for gate in self.graph.nodes_topologically_sorted():
            gate.forward()
        return loss # the final gate in the graph outputs the loss
    def backward():
        for gate in reversed(self.graph.nodes_topologically_sorted()):
            gate.backward() # little piece of backprop (chain rule applied)
        return inputs_gradients
```

Example: PyTorch Autograd Functions



(x,y,z are scalars)

```
class Multiply(torch.autograd.Function):
  @staticmethod
  def forward(ctx, x, y):
    ctx.save_for_backward(x, y)
    z = x * y
    return z
  @staticmethod
  def backward(ctx, grad_z):
    x, y = ctx.saved_tensors
    grad_x = y * grad_z   # dz/dx * dL/dz
    grad_y = x * grad_z   # dz/dy * dL/dz
    return grad_x, grad_y
```

Need to stash some values for use in backward

Upstream gradient

Multiply upstream and local gradients

Scalar Derivatives

$$x \in \mathbb{R}, y \in \mathbb{R}$$

Regular derivative:

$$\frac{\partial y}{\partial x} \in \mathbb{R}$$

If x changes by a small amount, how much will y change?

Vector Derivatives

$x \in \mathbb{R}, y \in \mathbb{R}$

Regular derivative:

$$\frac{\partial y}{\partial x} \in \mathbb{R}$$

If x changes by a small amount, how much will y change?

$x \in \mathbb{R}^N, y \in \mathbb{R}$

Derivative is **Gradient**:

$$\frac{\partial y}{\partial x} \in \mathbb{R}^N,$$

$$\left(\frac{\partial y}{\partial x}\right)_i = \frac{\partial y}{\partial x_i}$$

For each element of x, if it changes by a small amount then how much will y change?

Vector Derivatives

$x \in \mathbb{R}, y \in \mathbb{R}$

Regular derivative:

$$\frac{\partial y}{\partial x} \in \mathbb{R}$$

If x changes by a small amount, how much will y change?

$x \in \mathbb{R}^N, y \in \mathbb{R}$

Derivative is **Gradient**:

$$\frac{\partial y}{\partial x} \in \mathbb{R}^N,$$

$$\left(\frac{\partial y}{\partial x}\right)_i = \frac{\partial y}{\partial x_i}$$

For each element of x, if it changes by a small amount then how much will y change?

$x \in \mathbb{R}^N, y \in \mathbb{R}^M$

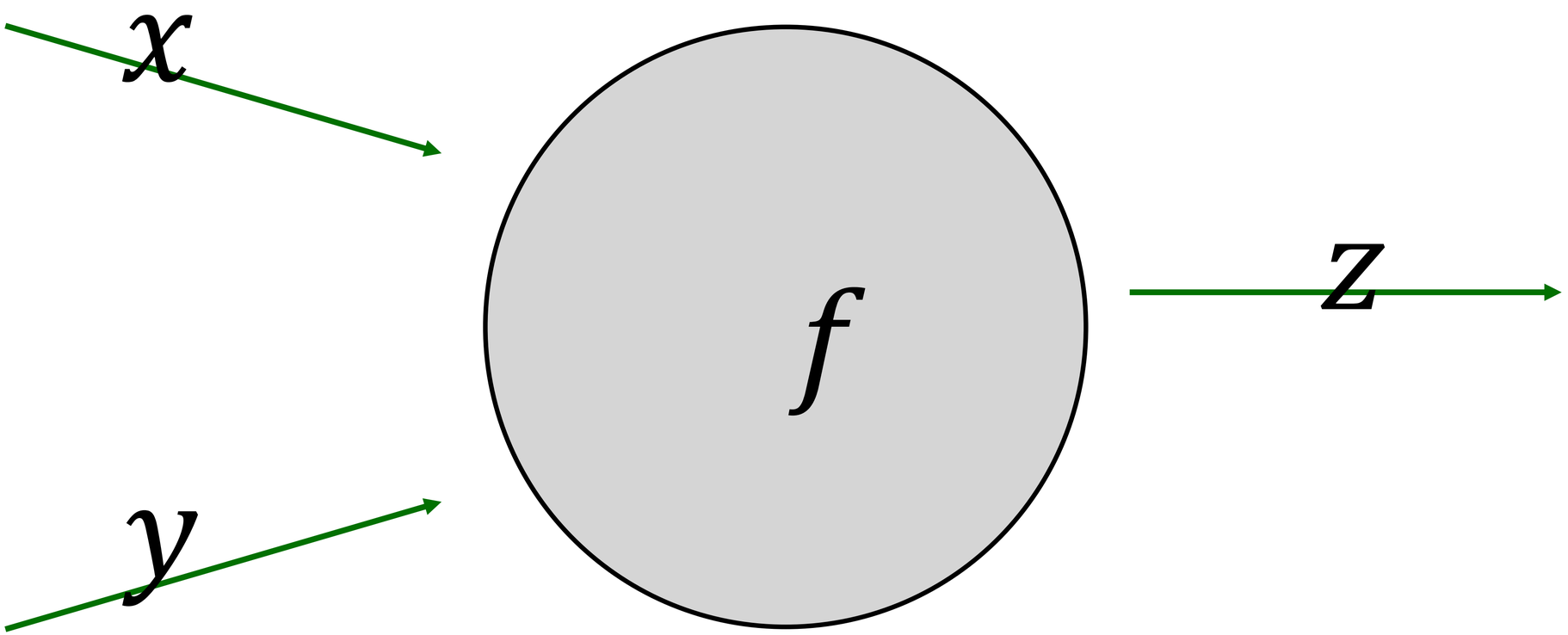
Derivative is **Jacobian**:

$$\frac{\partial y}{\partial x} \in \mathbb{R}^{N \times M}$$

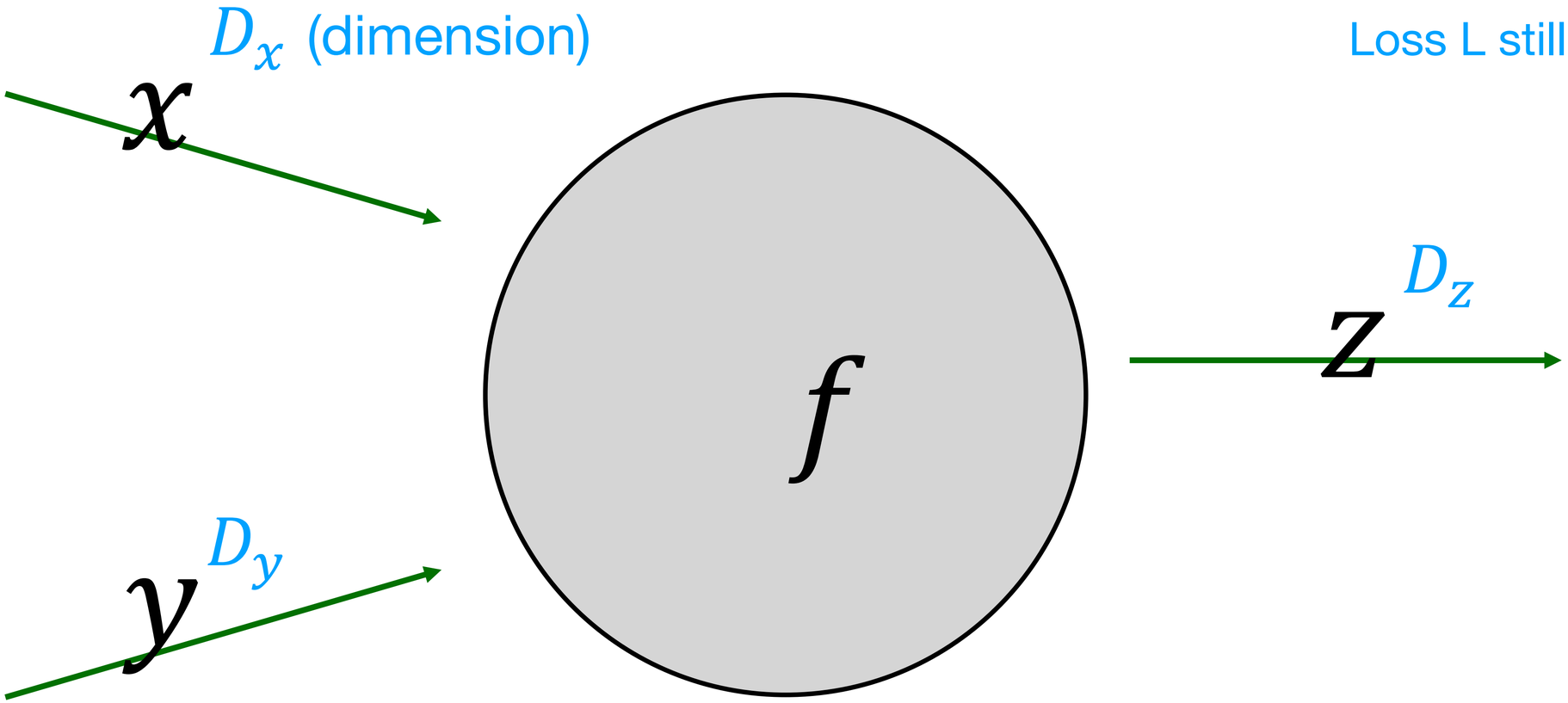
$$\left(\frac{\partial y}{\partial x}\right)_{i,j} = \frac{\partial y_j}{\partial x_i}$$

For each element of x, if it changes by a small amount then how much will each element of y change?

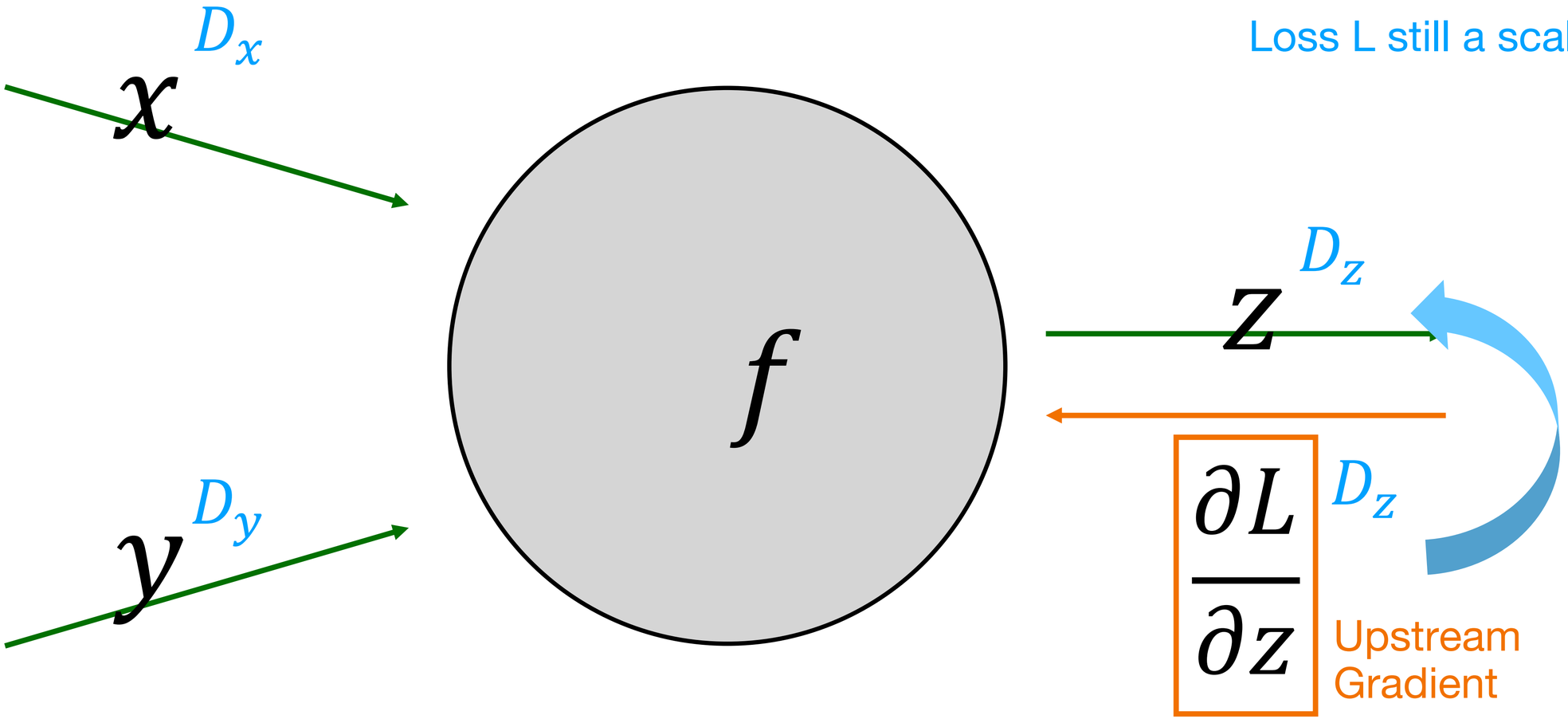
Backprop with Vectors: Dimensions



Backprop with Vectors: Dimensions



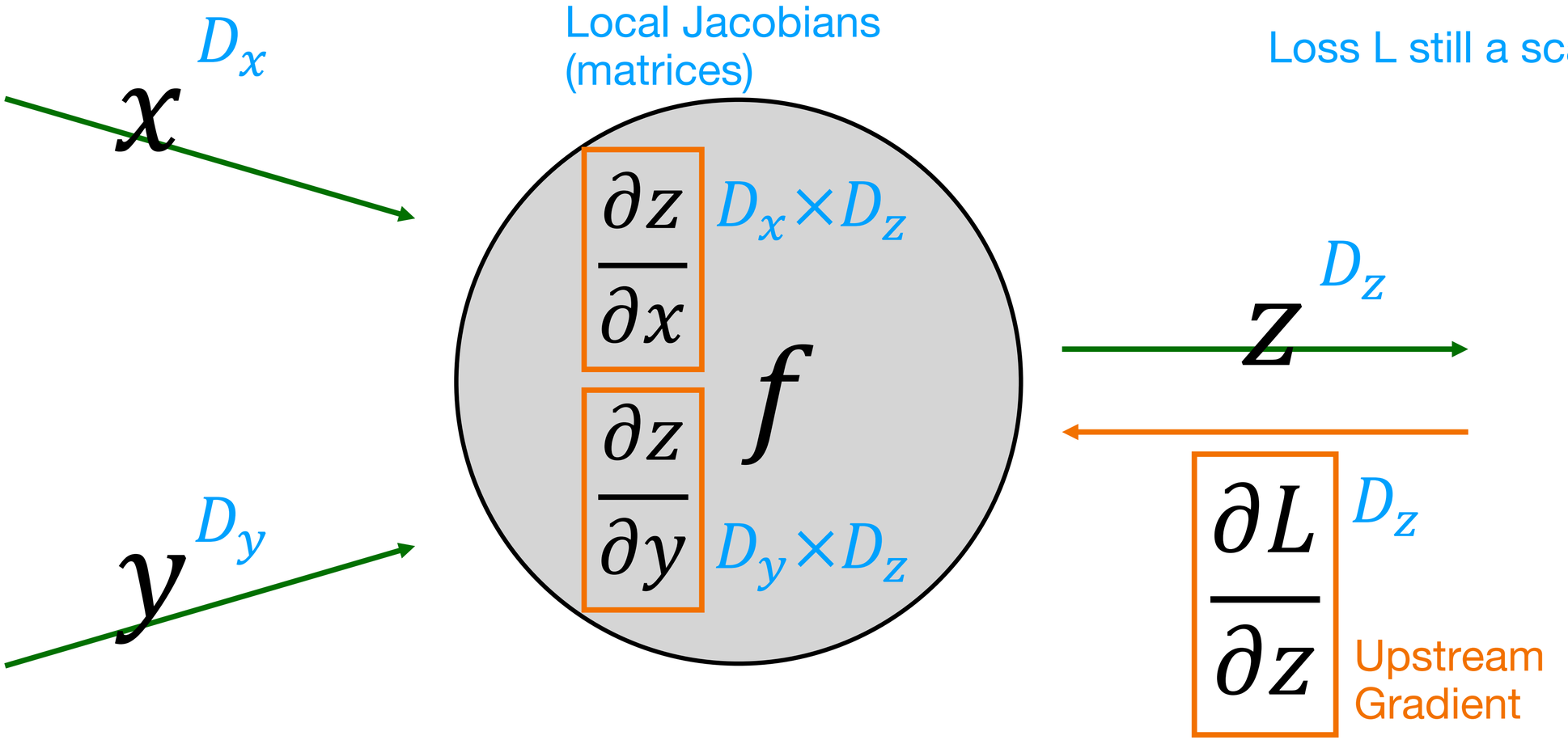
Backprop with Vectors: Dimensions



Loss L still a scalar!

For each element of z, how much does it influence L?

Backprop with Vectors: Dimensions



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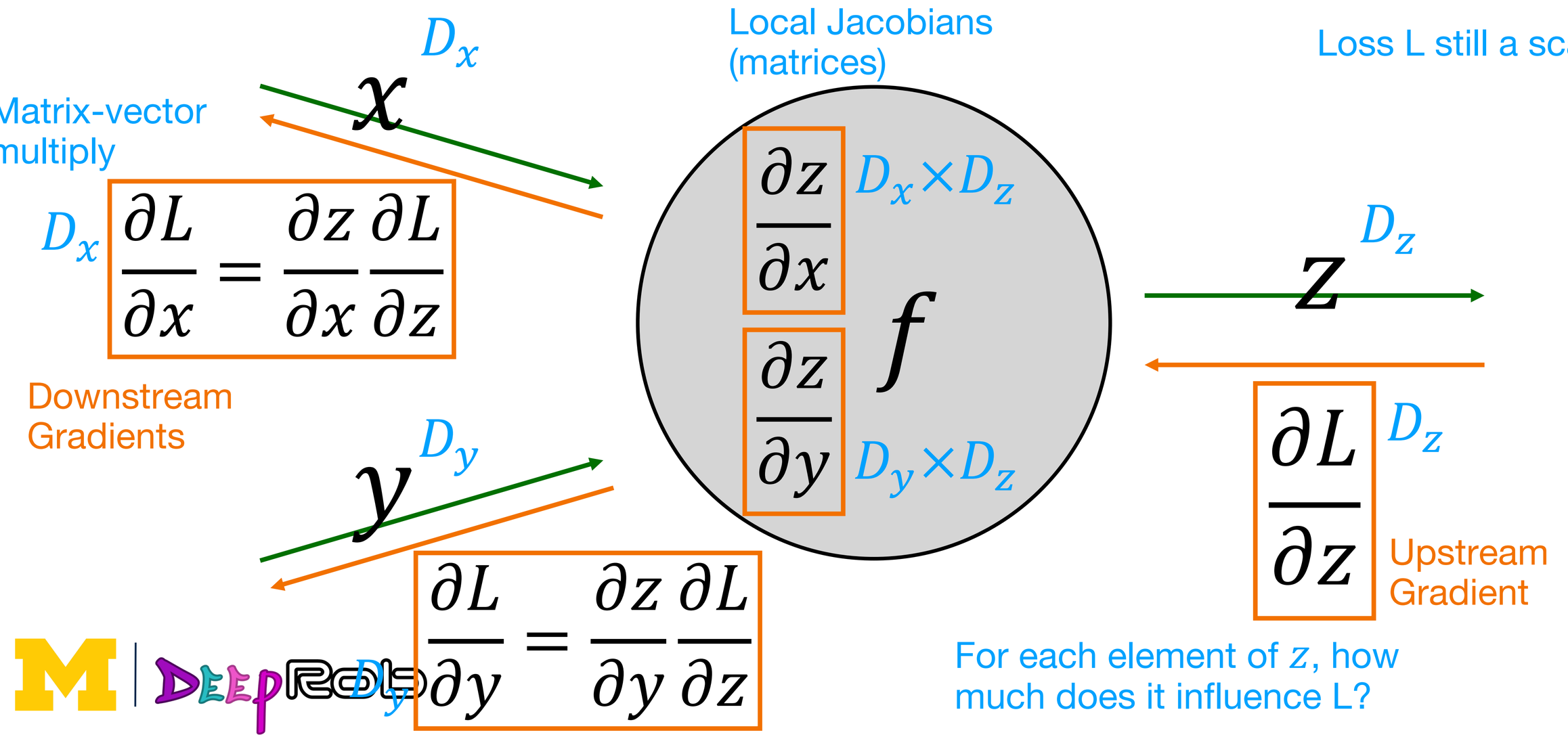
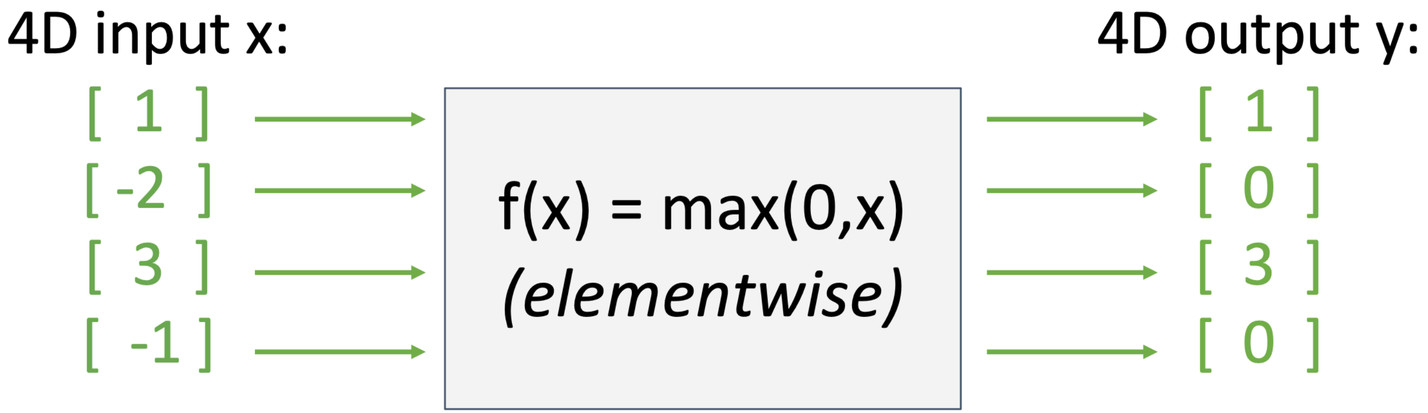
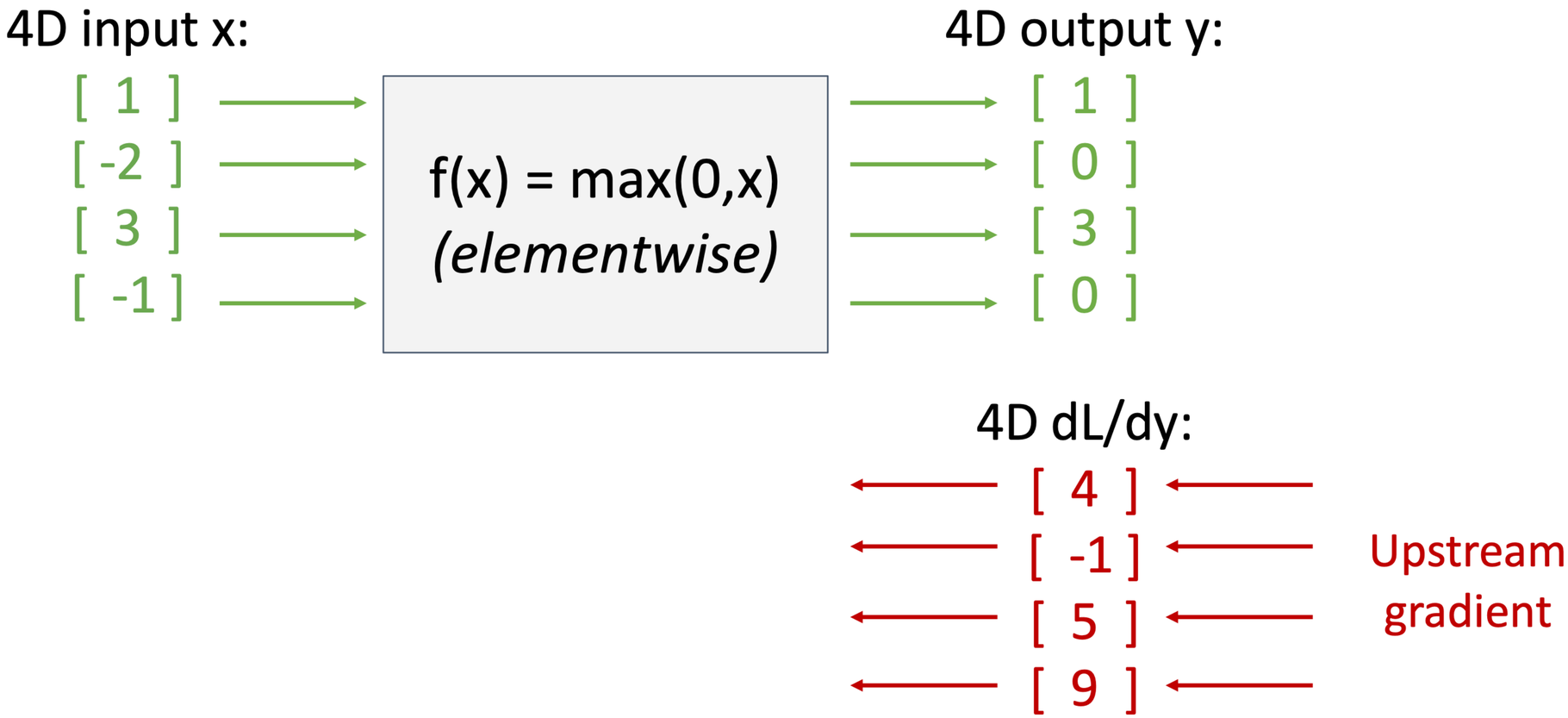
Backprop with Vectors: Dimensions



Backprop with Vectors



Backprop with Vectors



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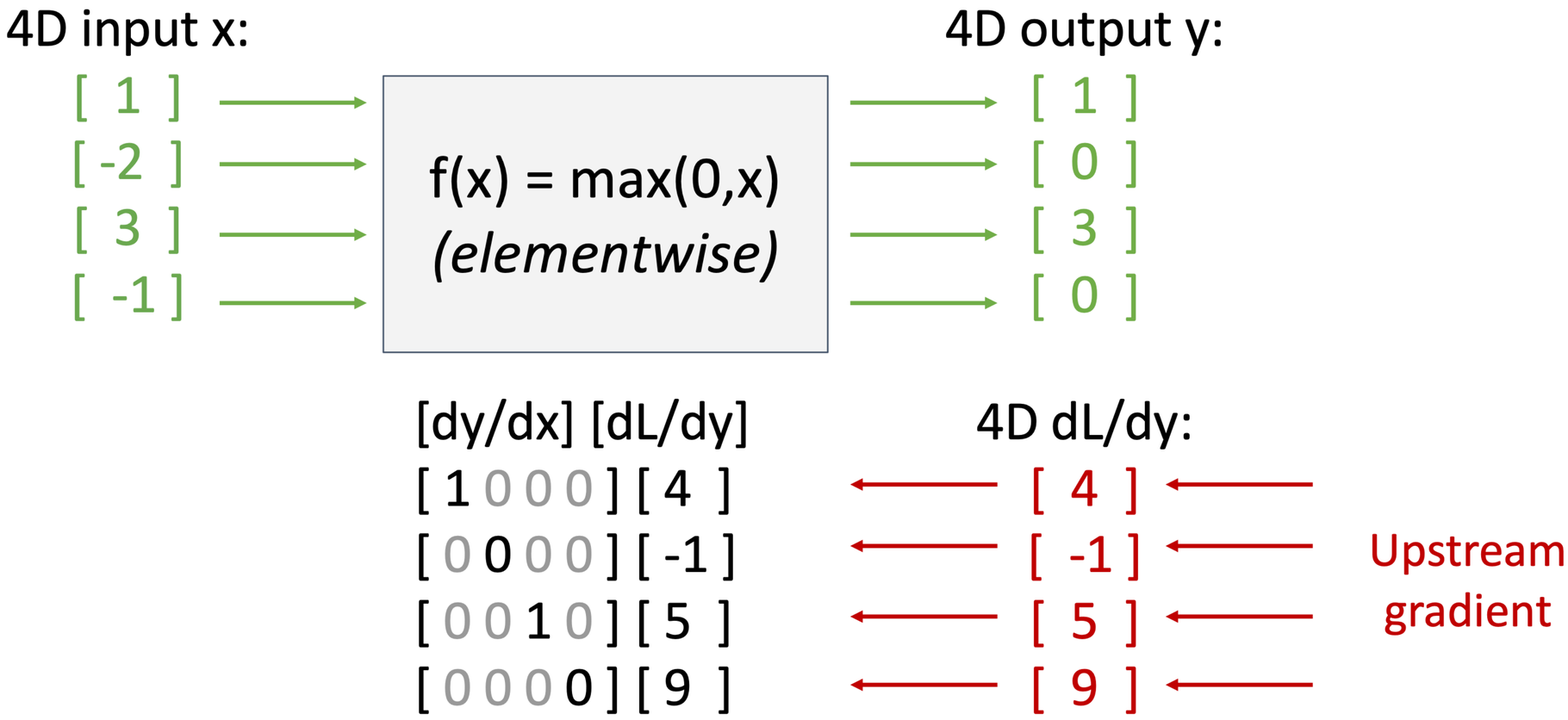
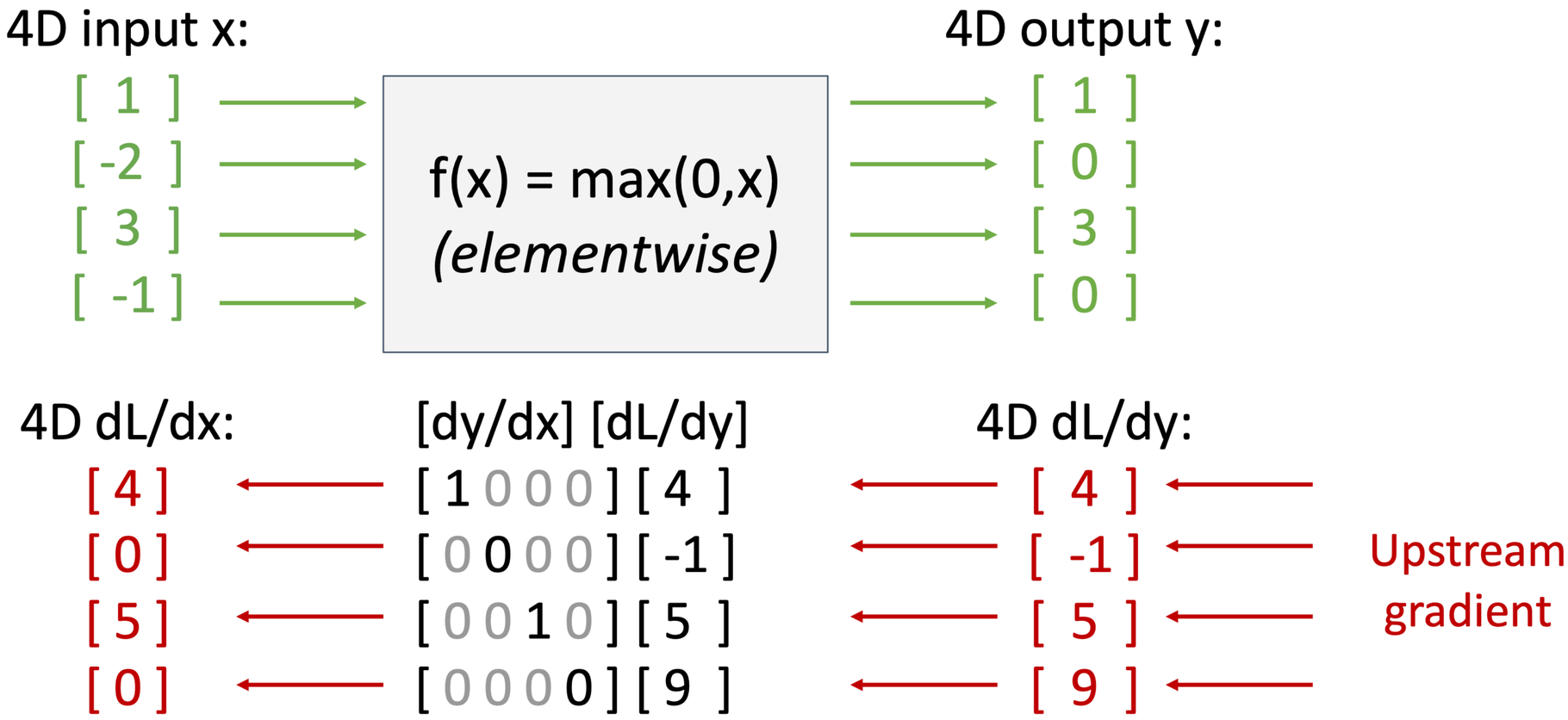
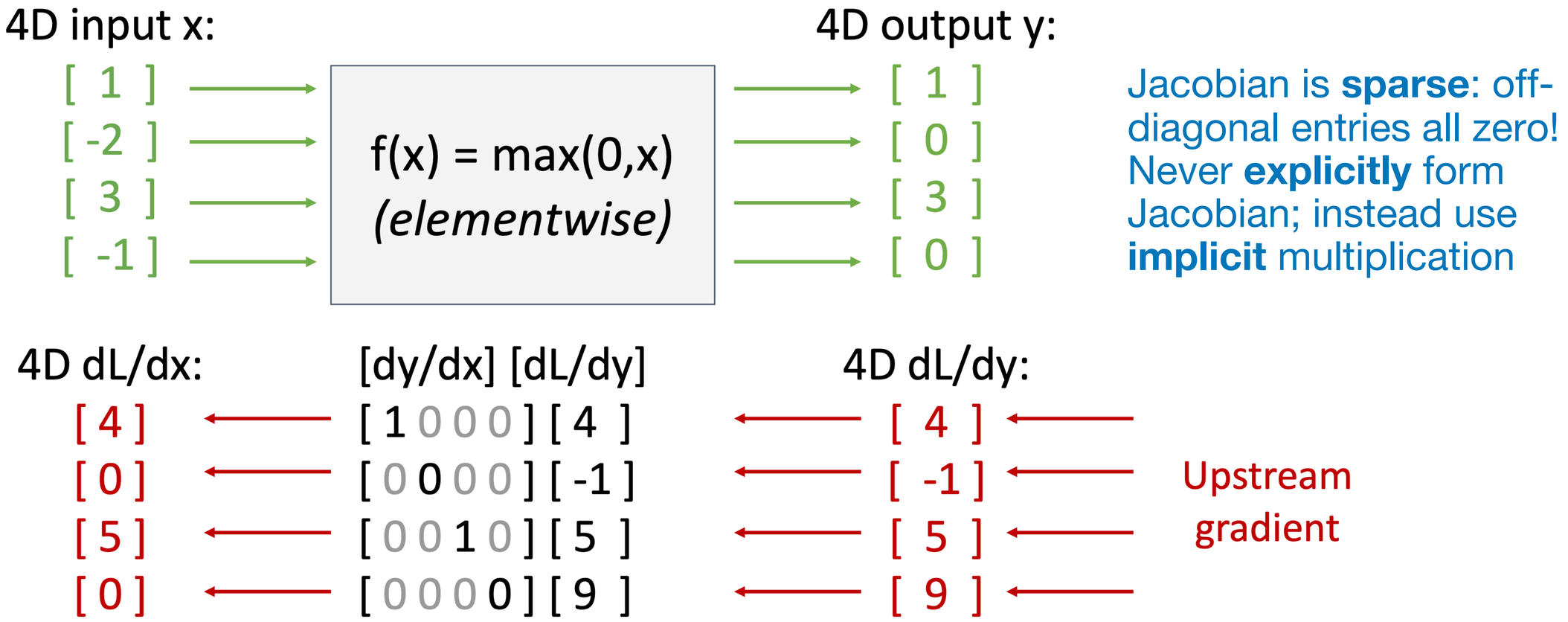


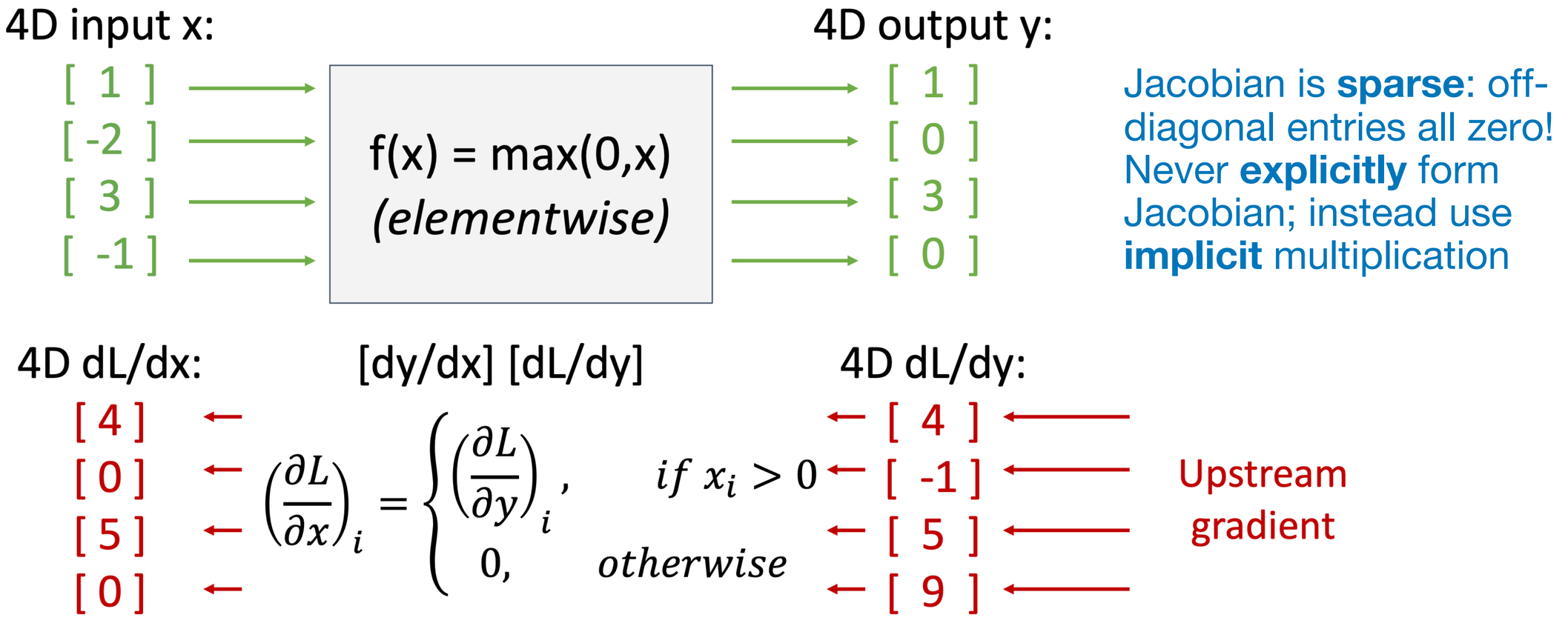
Backprop with Vectors



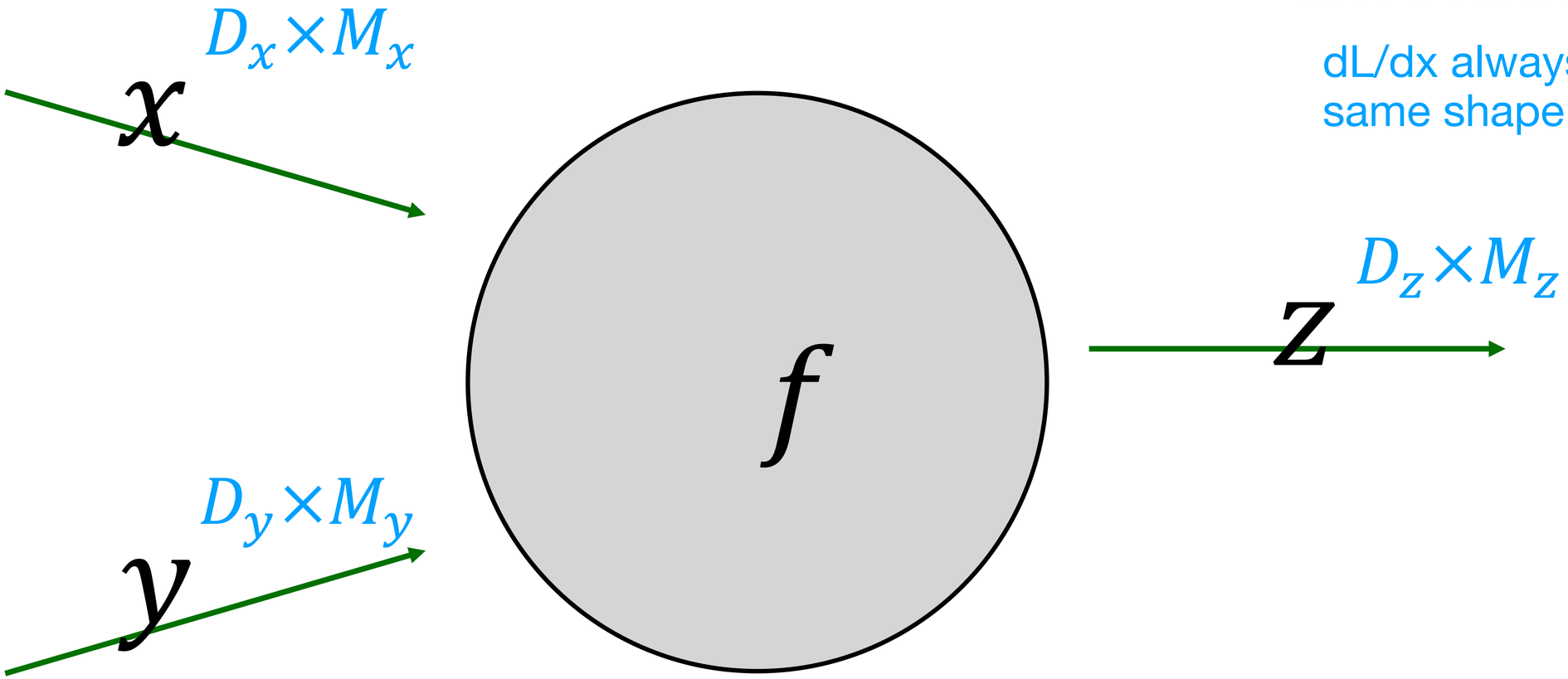
Backprop with Vectors



Backprop with Vectors



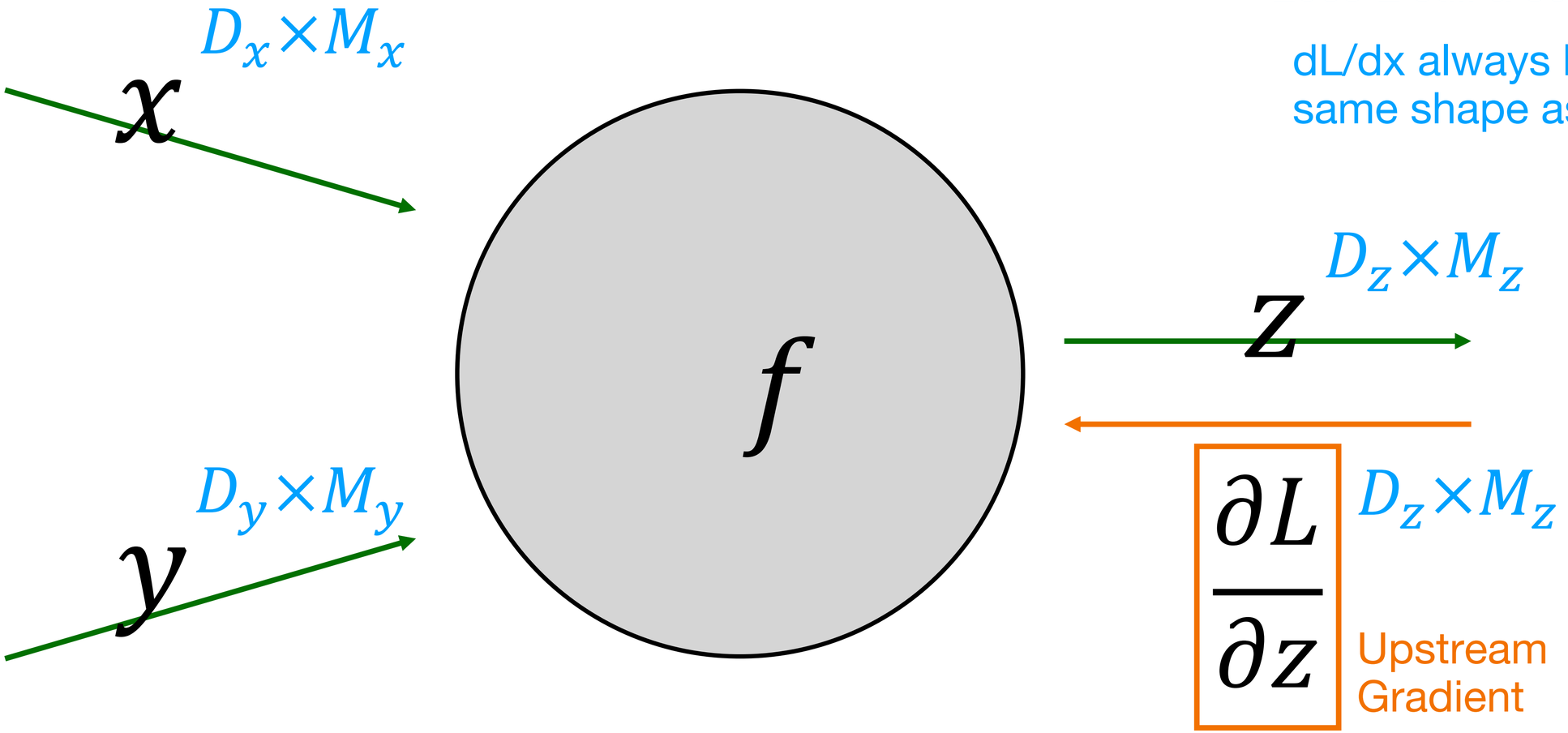
Backprop with Matrices (or Tensors)



Loss L still a scalar!

dL/dx always has the same shape as x!

Backprop with Matrices (or Tensors)



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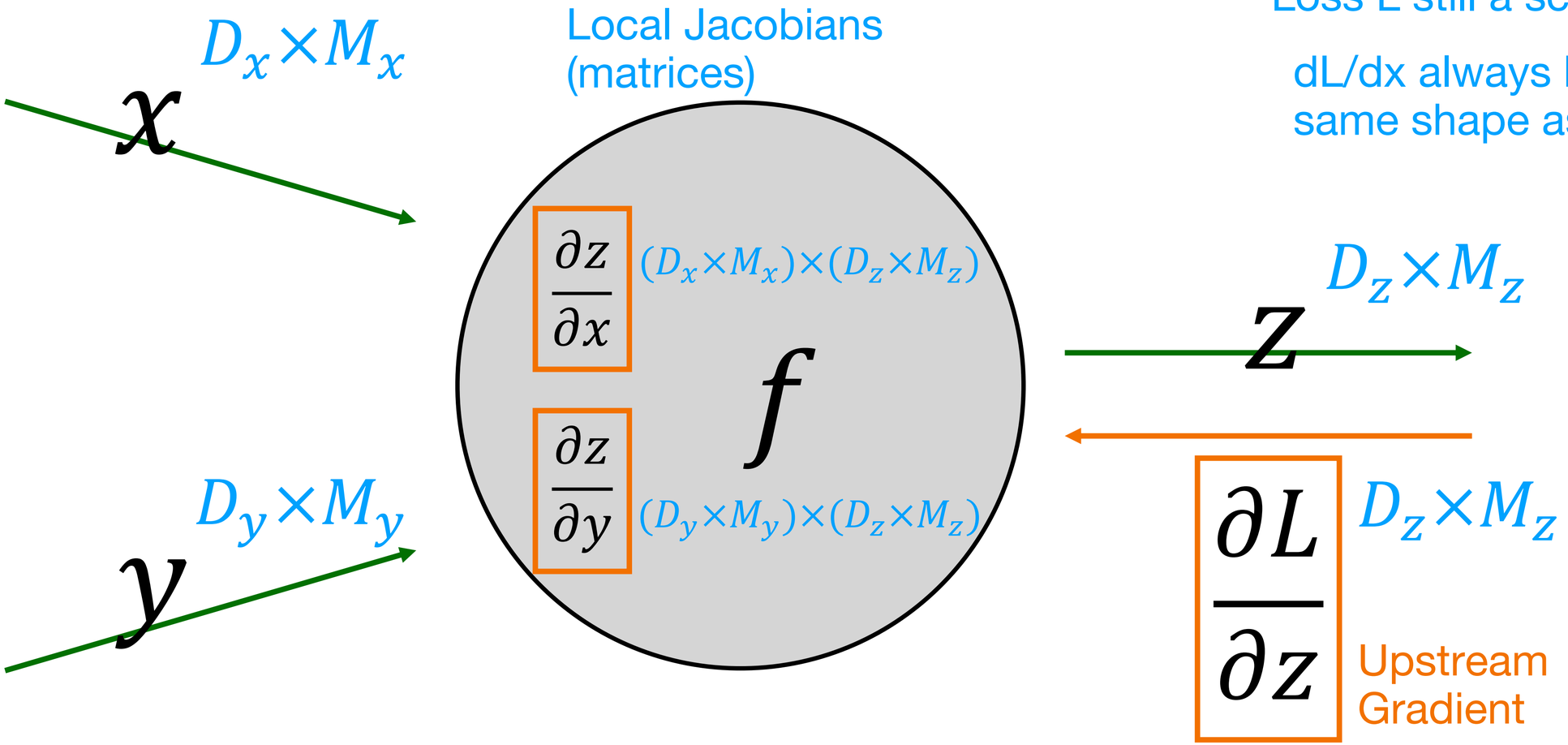
For each element of z, how much does it influence L?

Backprop with Matrices (or Tensors)



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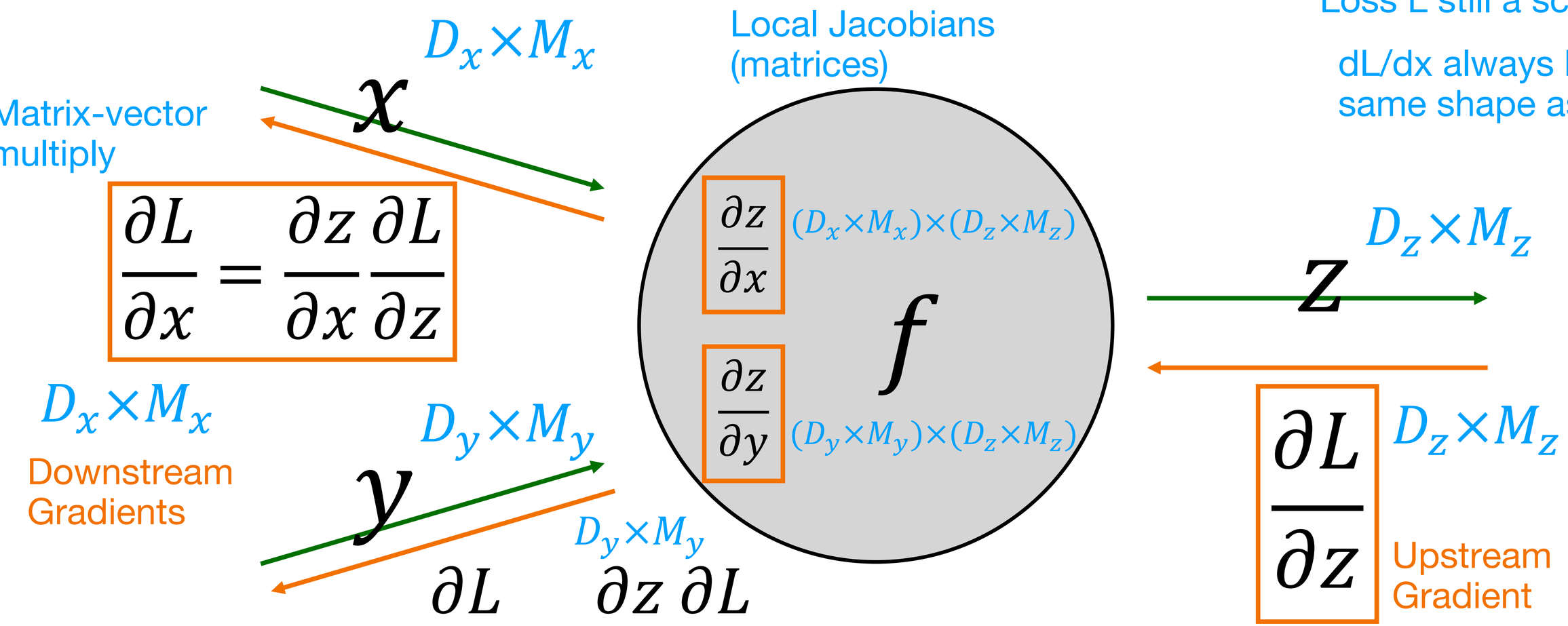

For each element of z, how much does it influence L?

Example: Matrix Multiplication

x: [N×D]

[2 1 -3]
[-3 4 2]

w: [D×M]

[3 2 1 -1]
[2 1 3 2]
[3 2 1 -2]

Matrix Multiply $y = xw$

$$y_{i,j} = \sum_k x_{i,k} w_{k,j}$$

y: [N×M]

[-1 -1 2 6]
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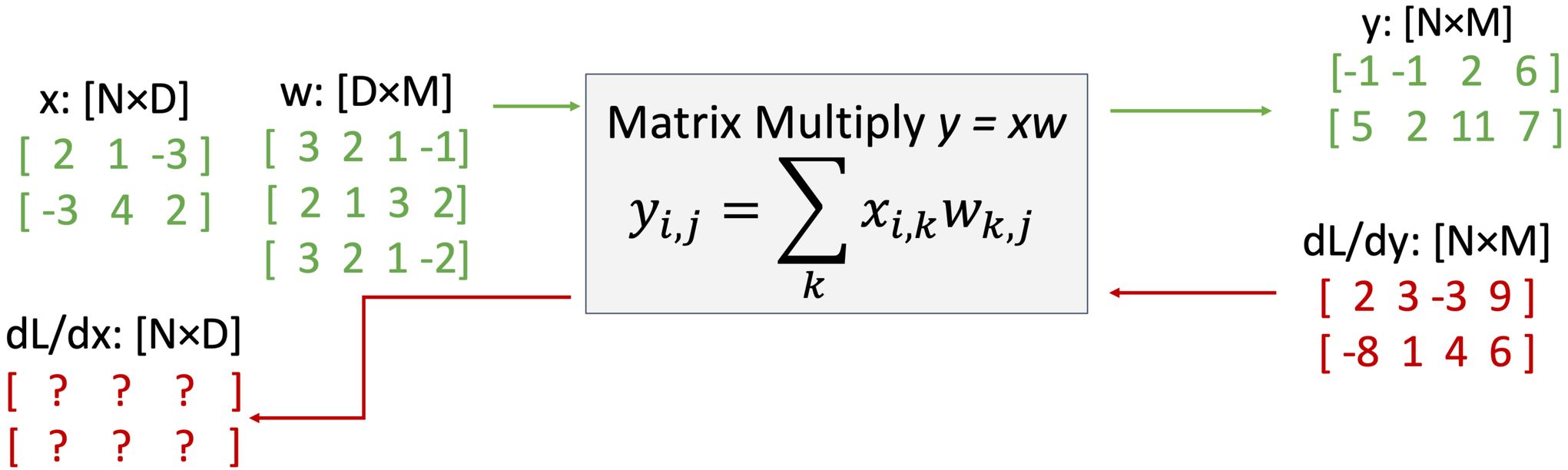
Example: Matrix Multiplication



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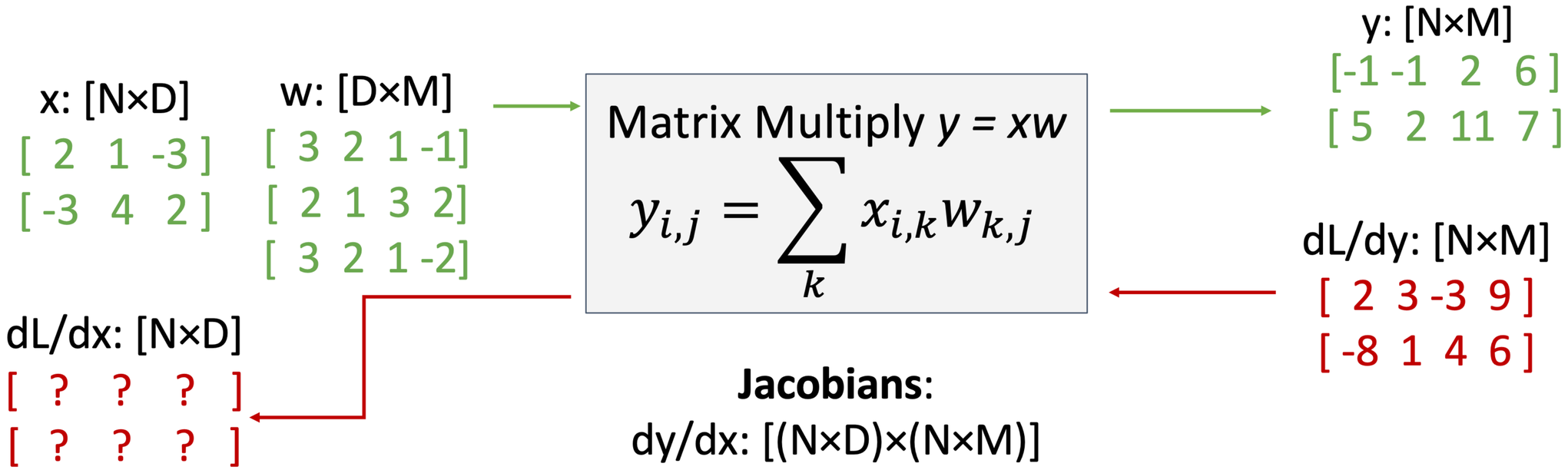


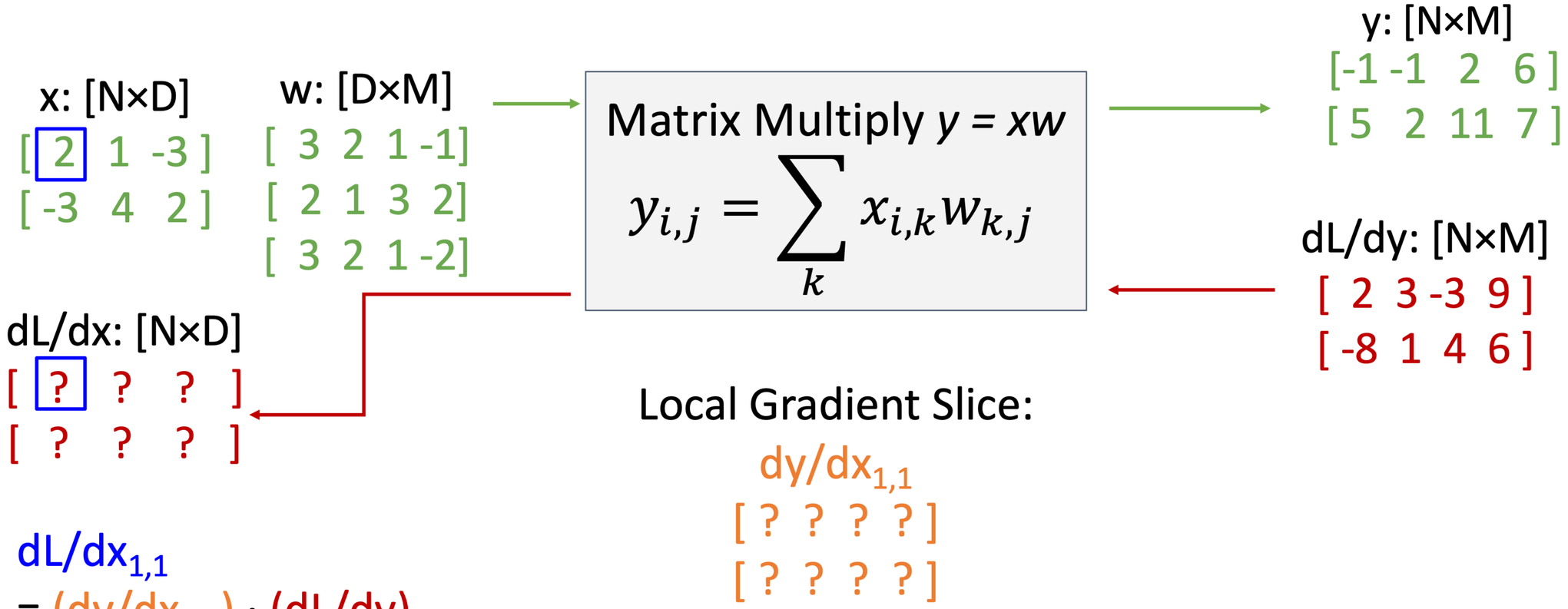
Jacobians:

dy/dx: [(N×D)×(N×M)]

dy/dw: [(D×M)×(N×M)]

For a neural net we may have
N=64, D=M=4096
Each Jacobian takes 256 GB of memory! Must work with them implicitly!

Example: Matrix Multiplication



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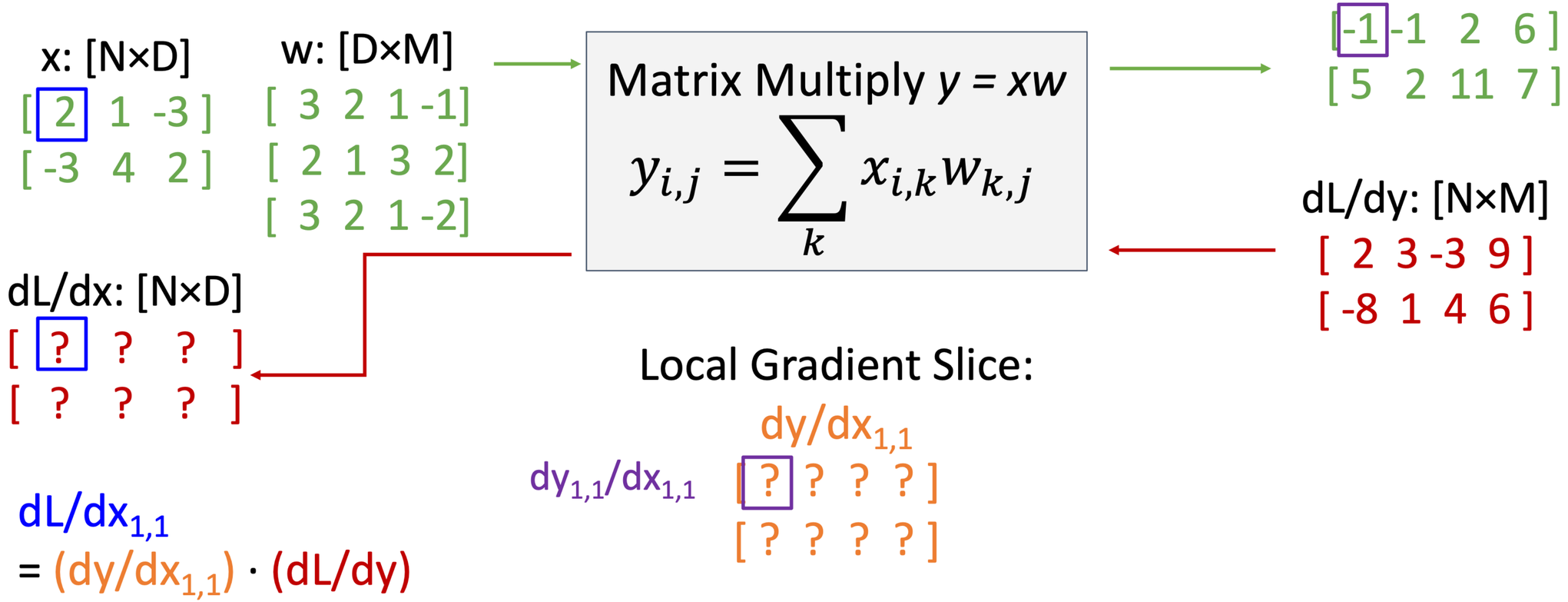

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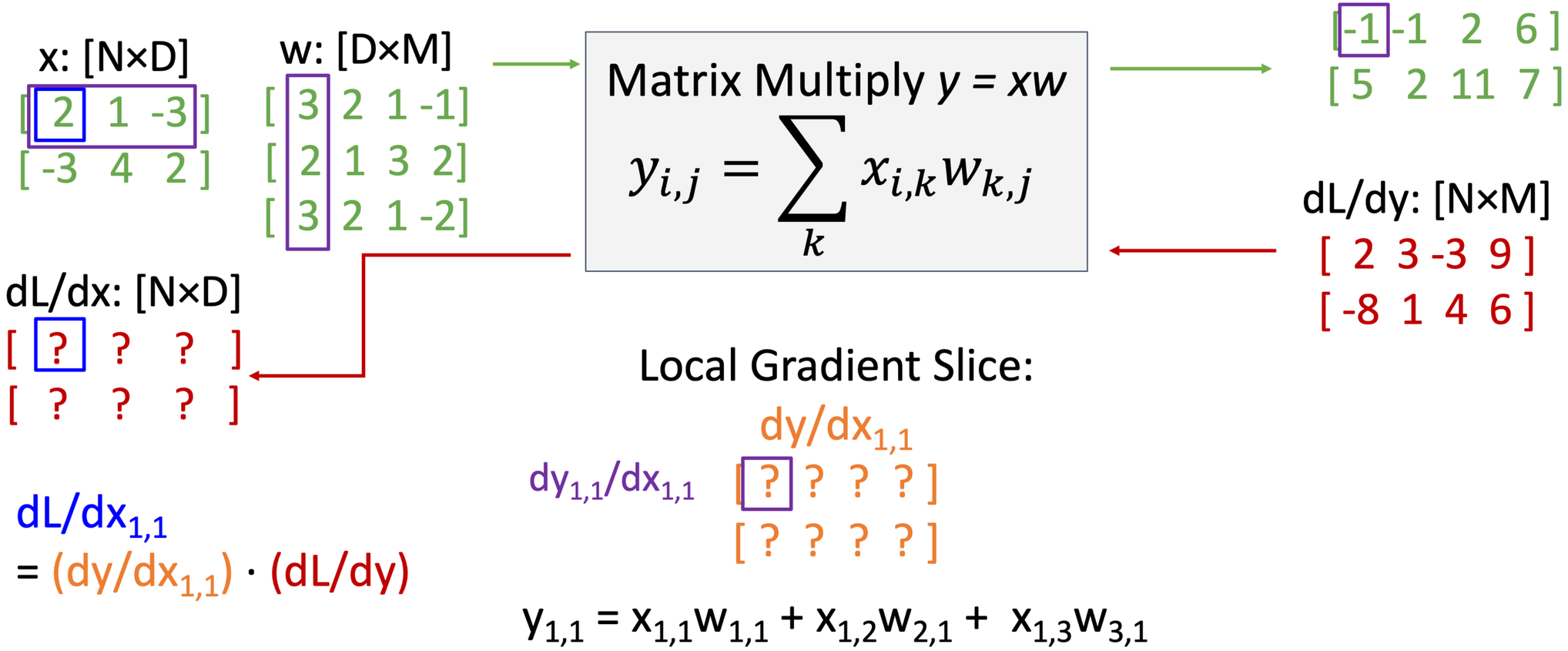

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[-1 -1 2 6]
[5 2 11 7]

dL/dy: [N×M]

[2 3 -3 9]
[-8 1 4 6]

dL/dx: [N×D]

[? ? ?]
[? ? ?]

$dL/dx_{1,1}$
$= (dy/dx_{1,1}) \cdot (dL/dy)$

Local Gradient Slice:

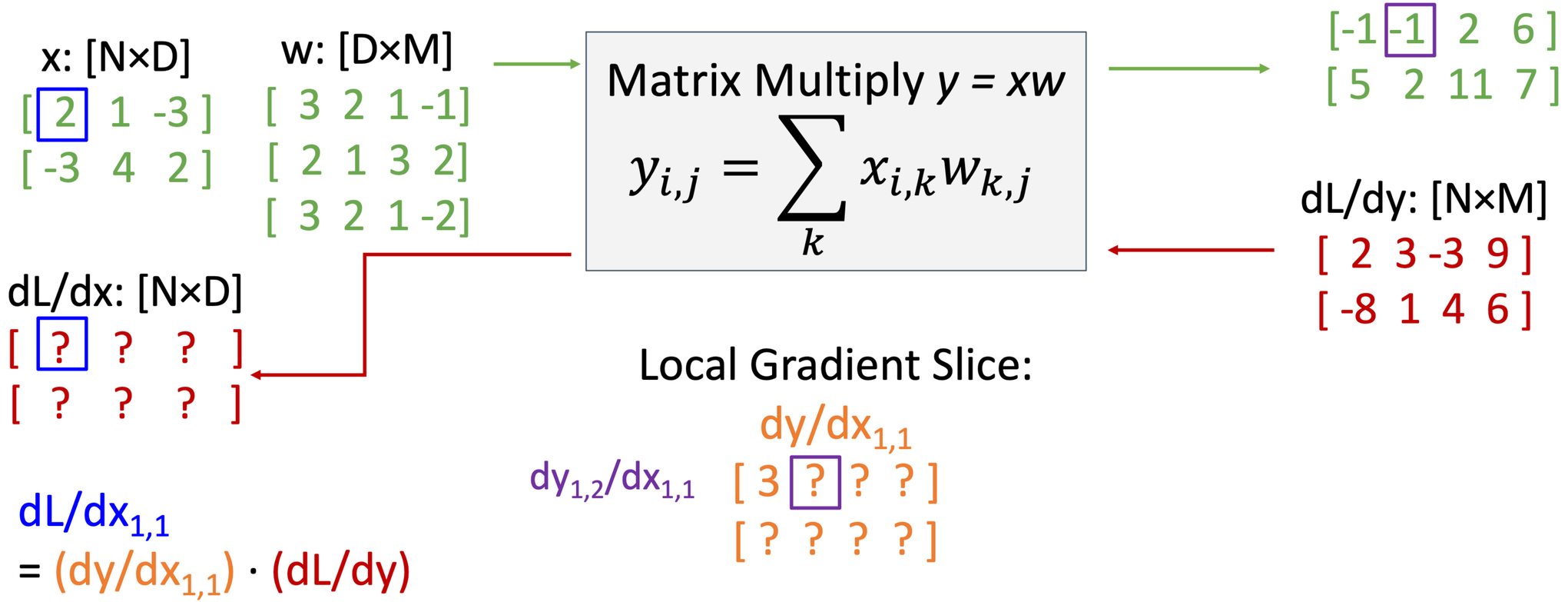
$dy/dx_{1,1}$

$dy_{1,1}/dx_{1,1}$ [3 ? ? ?]
[? ? ? ?]

$y_{1,1} = x_{1,1}w_{1,1} + x_{1,2}w_{2,1} + x_{1,3}w_{3,1}$

$\Rightarrow dy_{1,1}/dx_{1,1} = w_{1,1}$

Example: Matrix Multiplication



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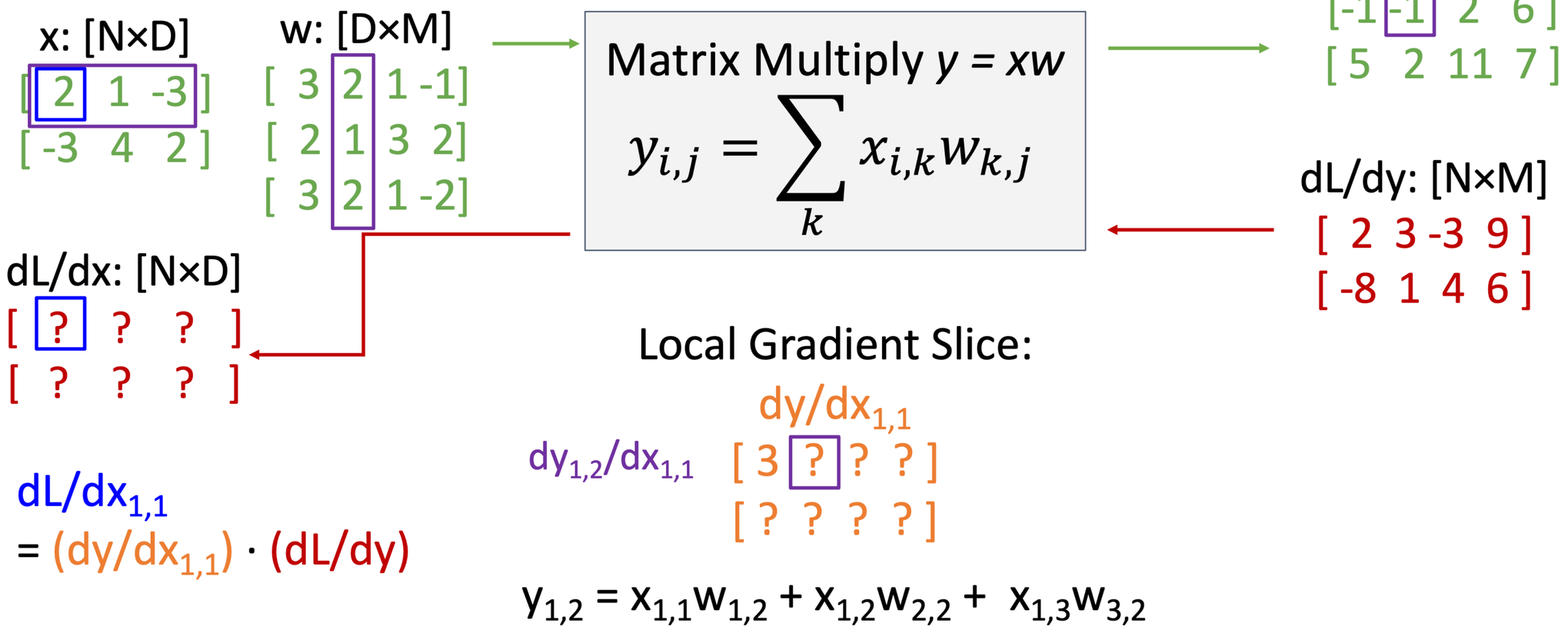
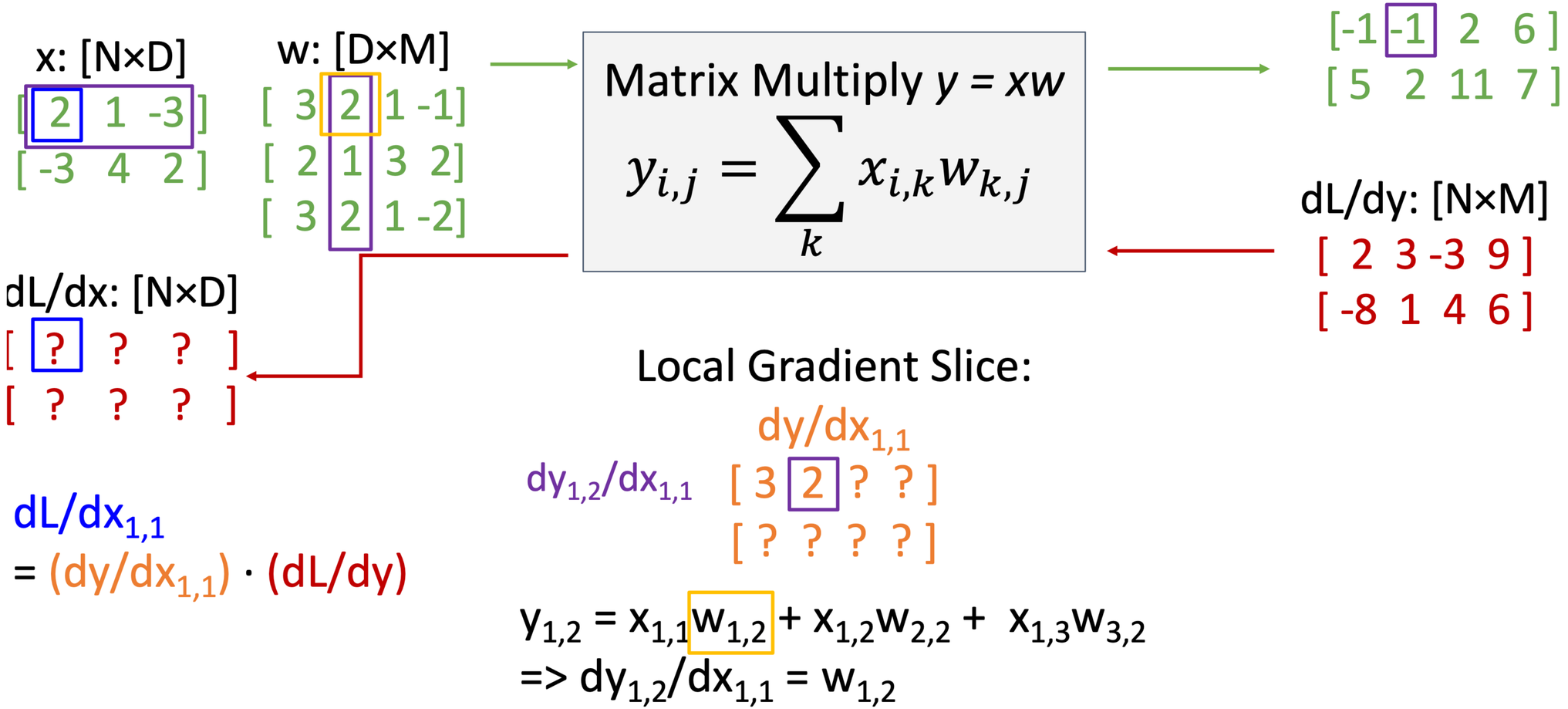


Example: Matrix Multiplication



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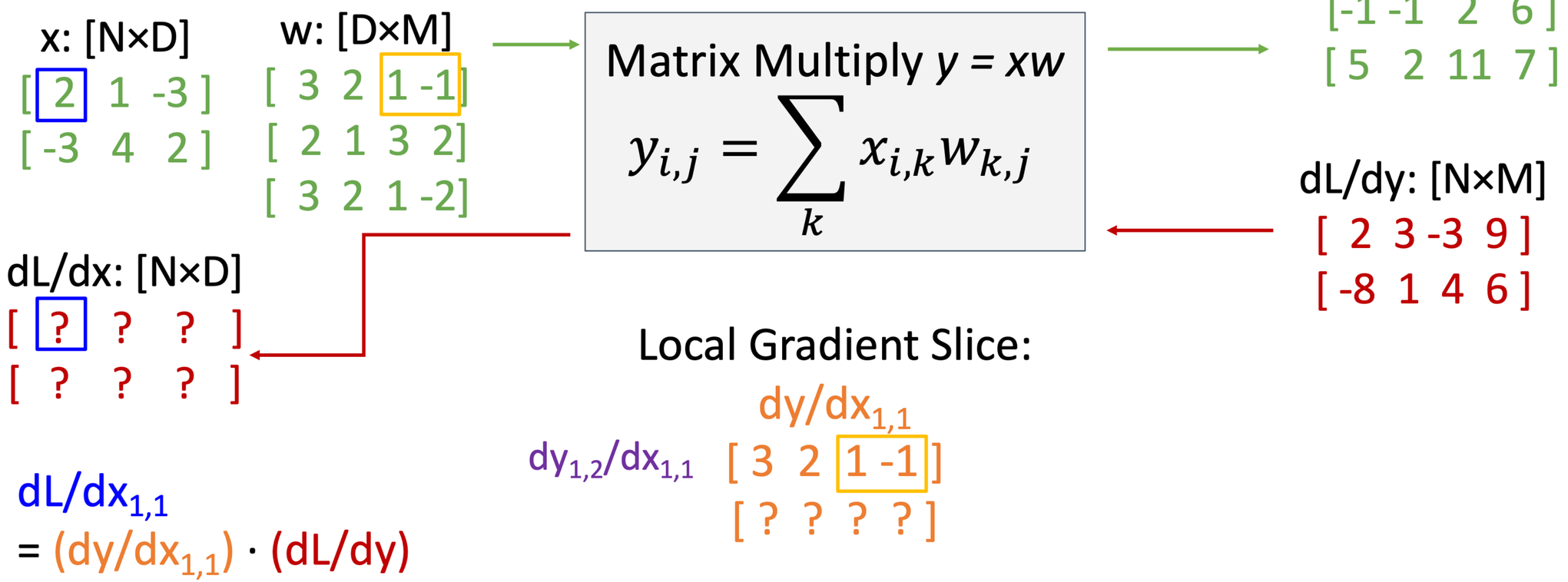

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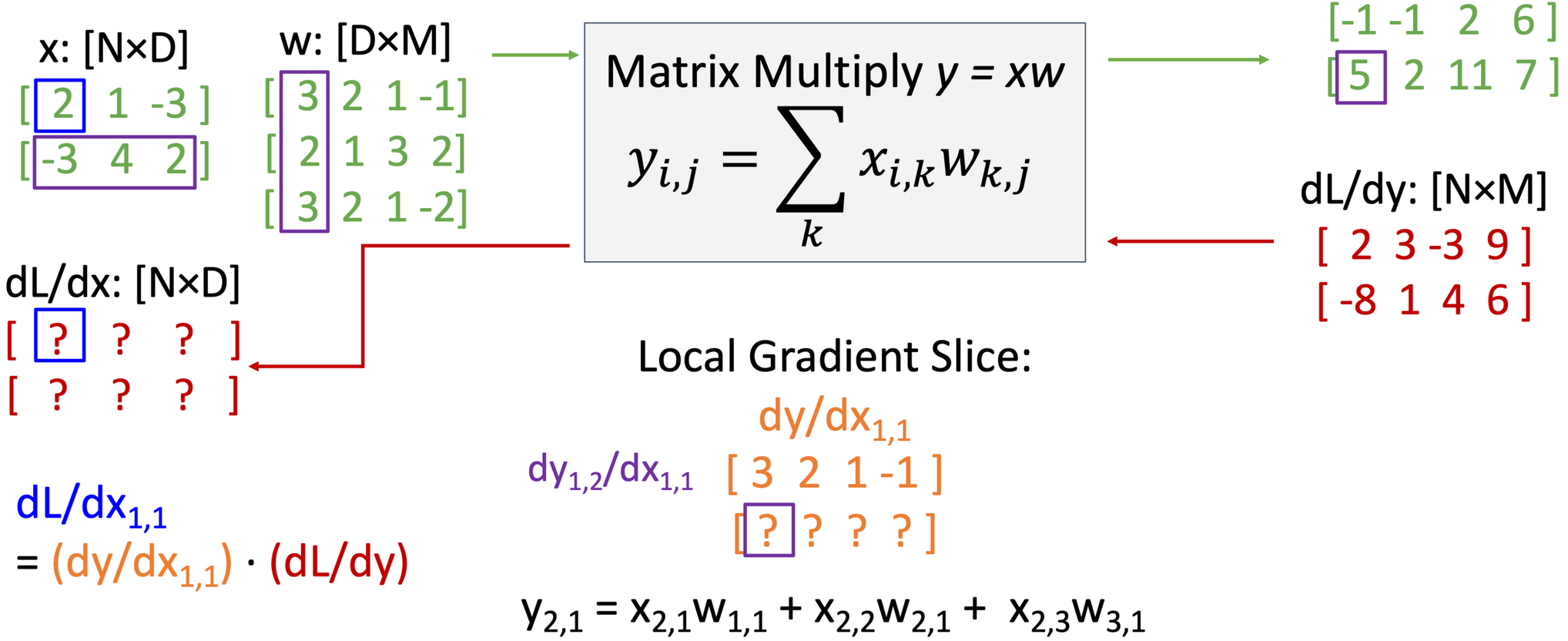
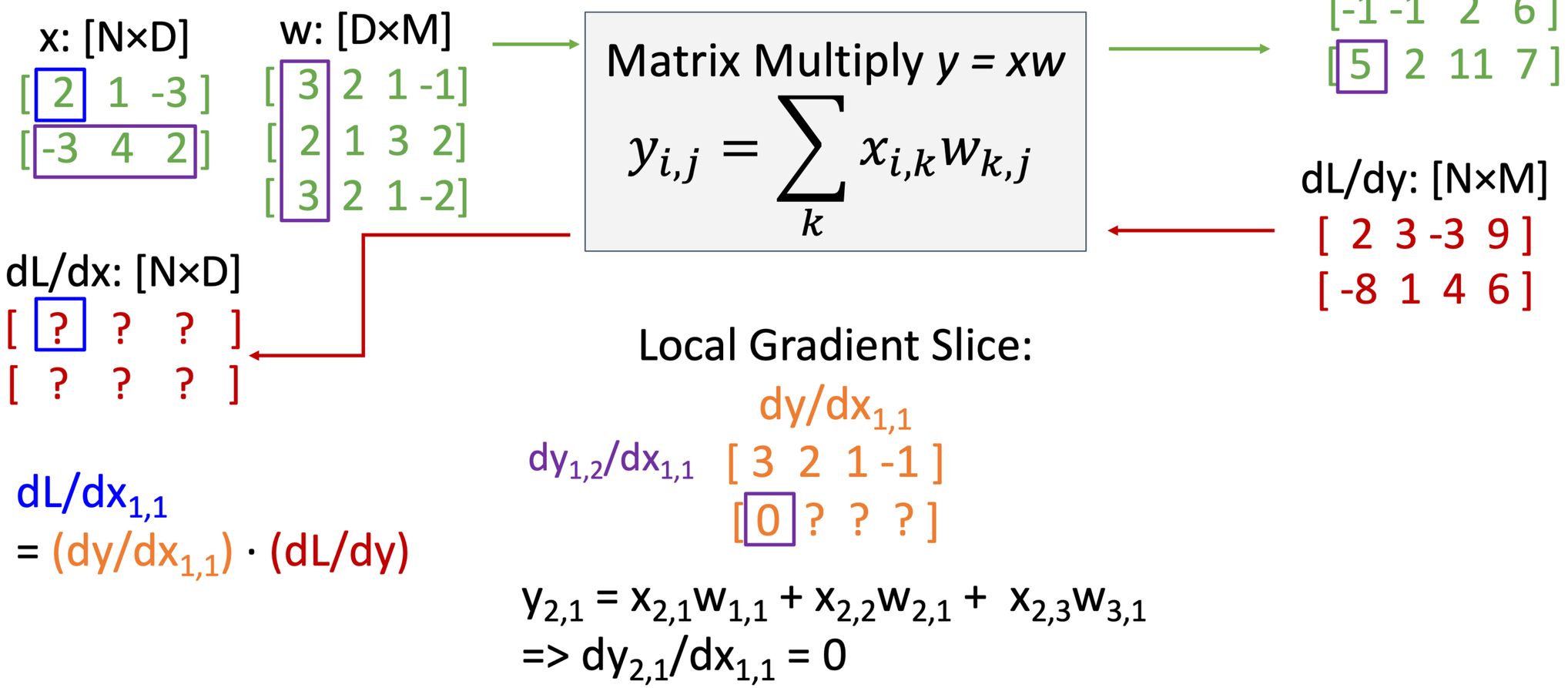
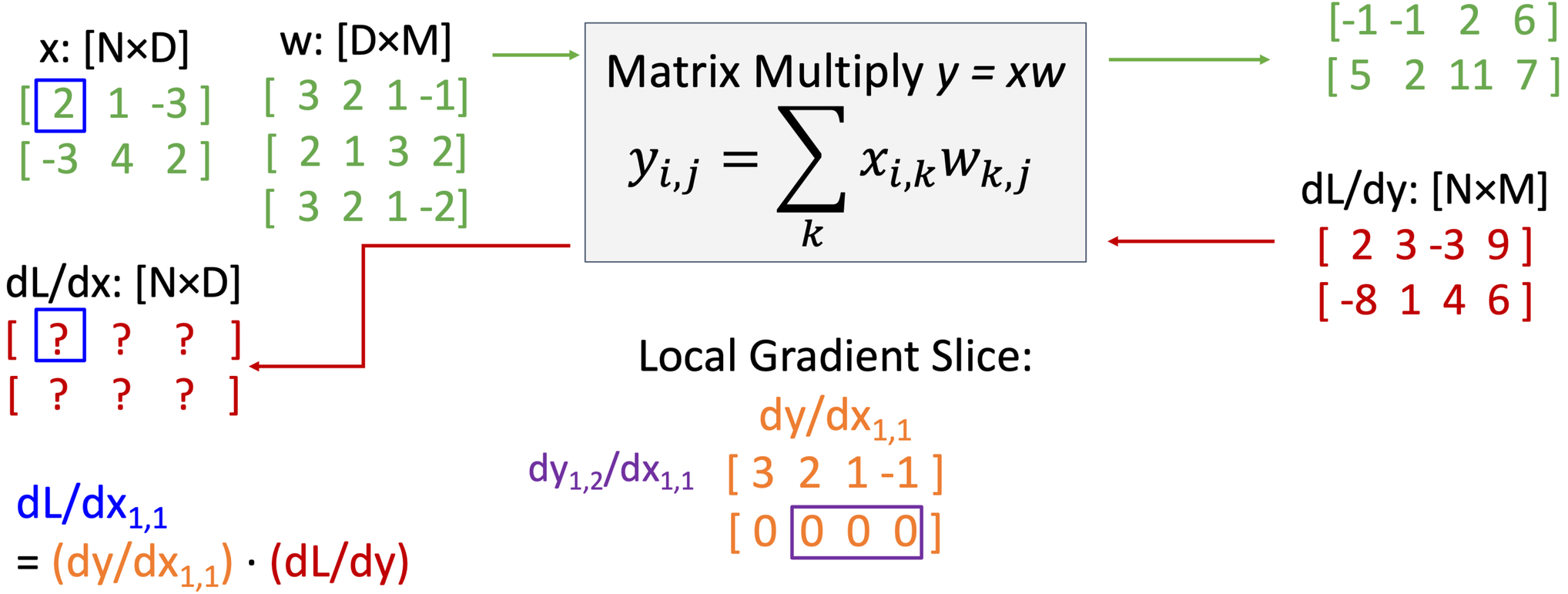


Example: Matrix Multiplication



Example: Matrix Multiplication



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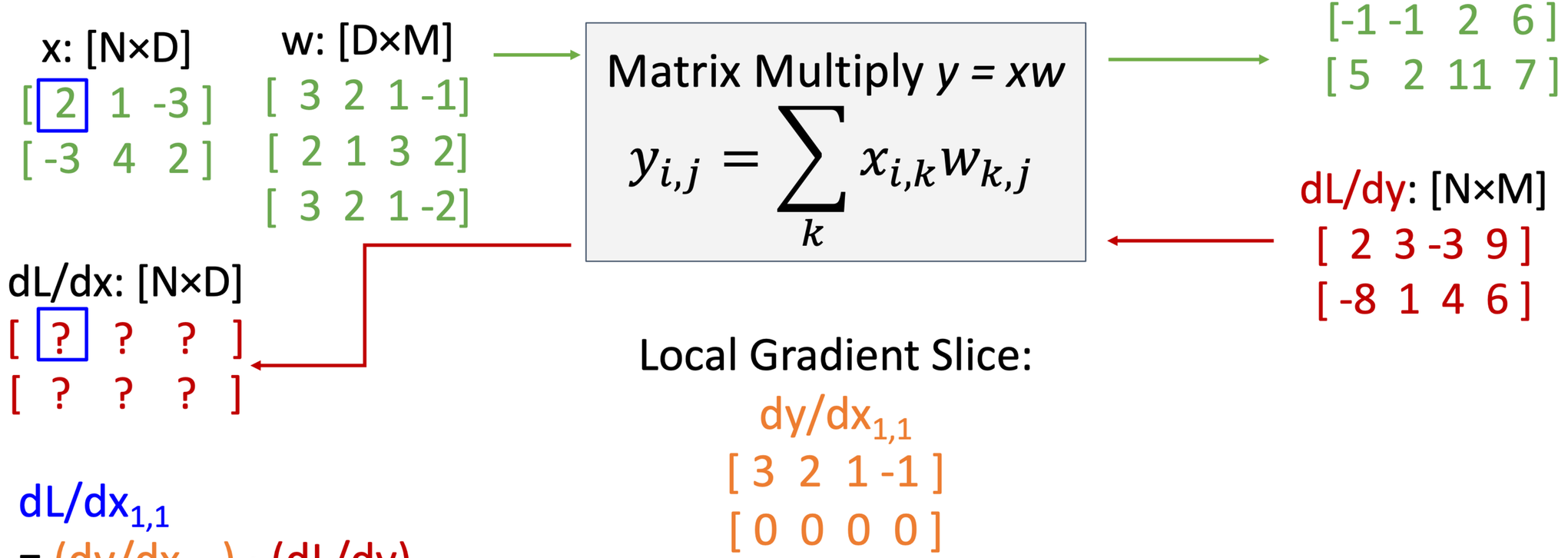
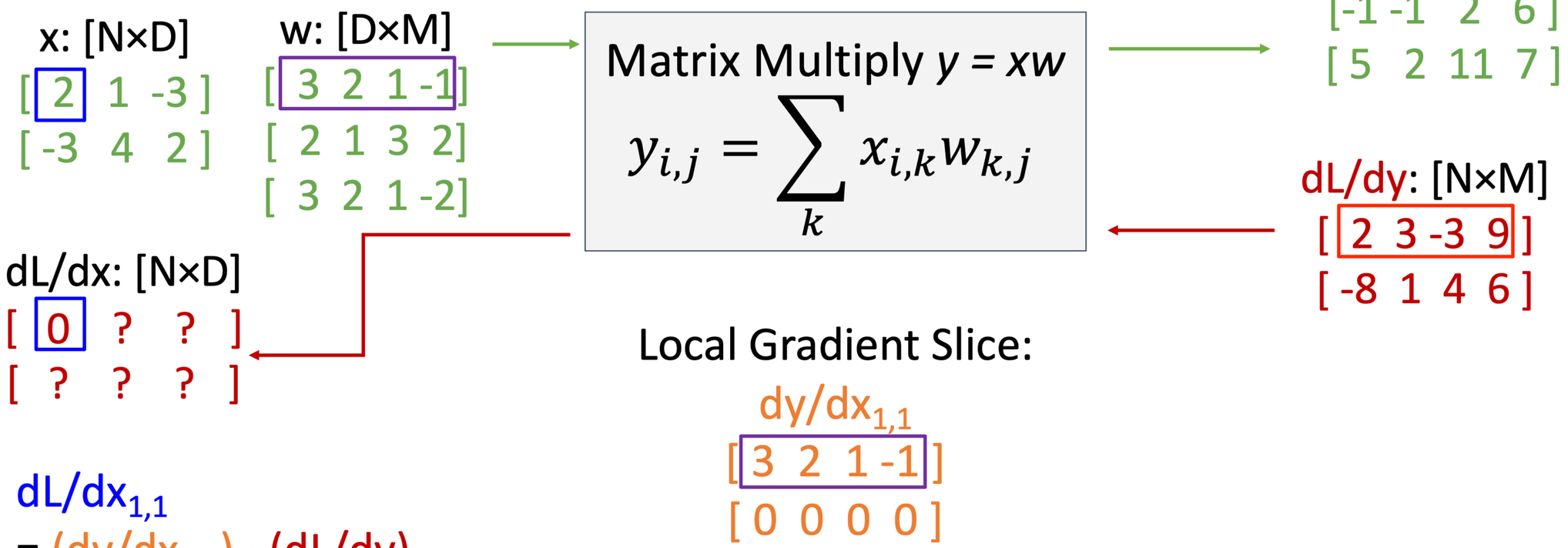
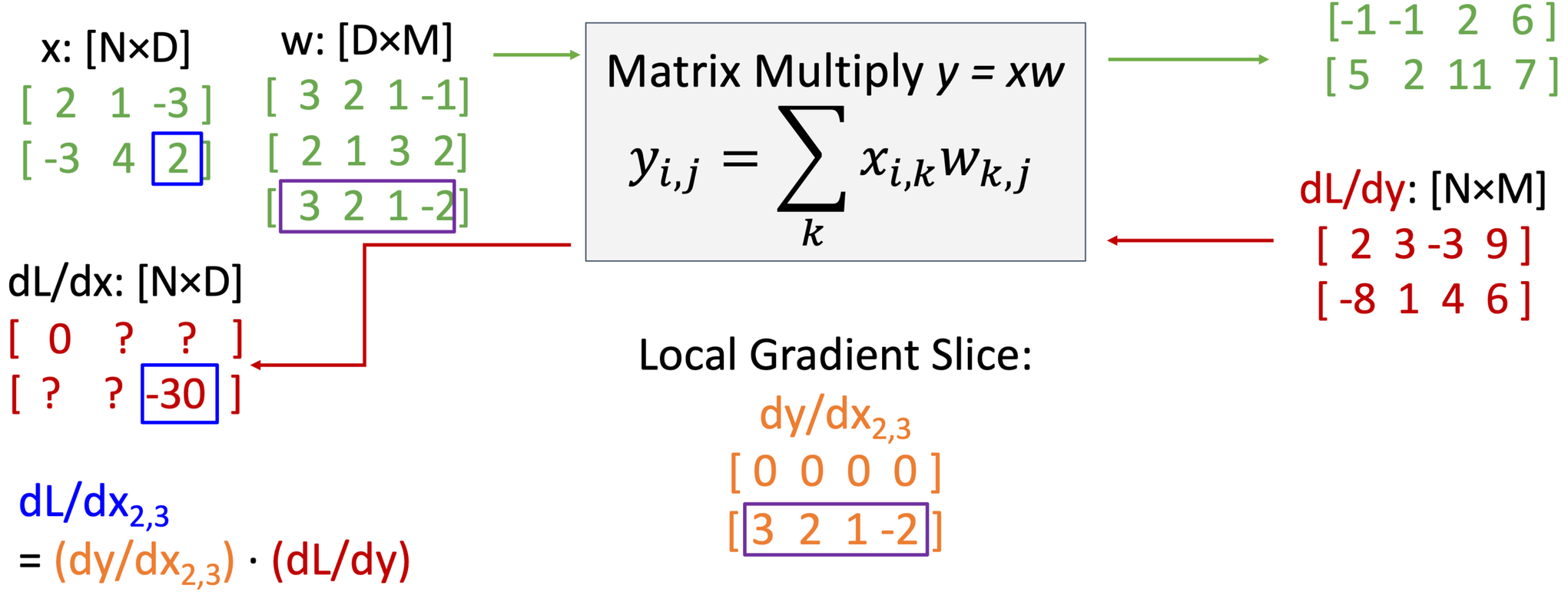


Example: Matrix Multiplication

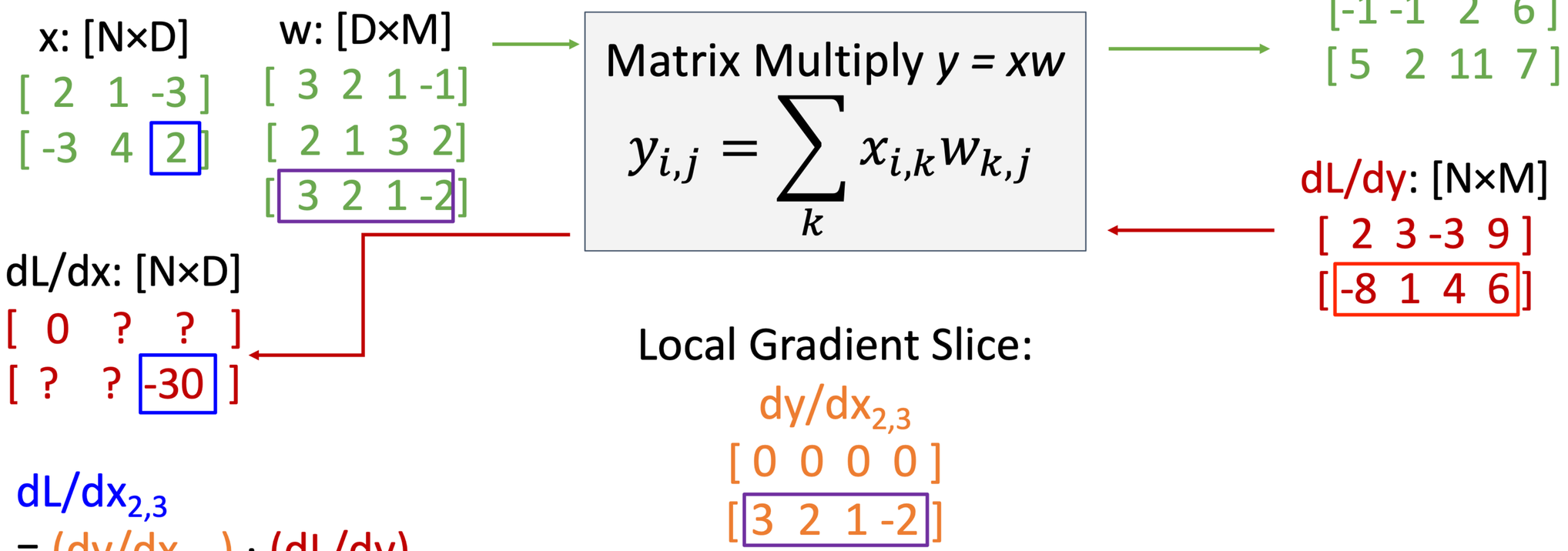


$dL/dx_{1,1}$
$= (dy/dx_{1,1}) \cdot (dL/dy)$
$= (w_{1,:}) \cdot (dL/dy_{1,:})$
$= 3*2 + 2*3 + 1*(-3) + (-1)*9 = 0$

Example: Matrix Multiplication



Example: Matrix Multiplication



$dL/dx_{2,3}$
$= (dy/dx_{2,3}) \cdot (dL/dy)$
$= (w_{3,:}) \cdot (dL/dy_{2,:})$
$= 3*(-8) + 2*1 + 1*4 + (-2)*6 = -30$

Example: Matrix Multiplication

x: [N×D]
[2 1 -3]
[-3 4 2]

w: [D×M]
[3 2 1 -1]
[2 1 3 2]
[3 2 1 -2]

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$$y_{i,j} = \sum_k x_{i,k} w_{k,j}$$

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[5 2 11 7]

dL/dy: [N×M]
[2 3 -3 9]
[-8 1 4 6]

dL/dx: [N×D]
[0 16 -9]
[-24 9 -30]

$dL/dx_{i,j}$
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Example: Matrix Multiplication

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[-8 1 4 6]

dL/dx: [N×D]
[0 16 -9]
[-24 9 -30]

$dL/dx = (dL/dy)\, w^T$

[N x D] [N x M] [M x D]

$dL/dx_{i,j}$
$= (dy/dx_{i,j}) \cdot (dL/dy)$
$= (w_{j,:}) \cdot (dL/dy_{i,:})$

Easy way to remember:
It's the only way the shapes work out!

Example: Matrix Multiplication

x: [N×D]
[2 1 -3]
[-3 4 2]

w: [D×M]
[3 2 1 -1]
[2 1 3 2]
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[-1 -1 2 6]
[5 2 11 7]

dL/dy: [N×M]
[2 3 -3 9]
[-8 1 4 6]

dL/dx: [N×D]
[0 16 -9]
[-24 9 -30]

$dL/dx = (dL/dy)\, w^T$

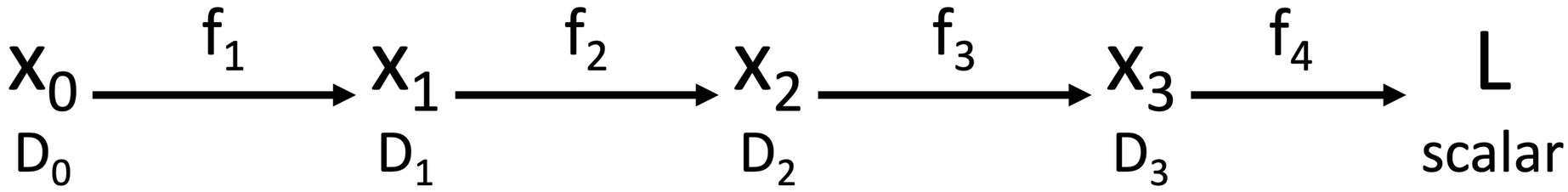
[N x D] [N x M] [M x D]

$dL/dw = x^T\, (dL/dy)$

[D x M] [D x N] [N x M]

Easy way to remember:
It's the only way the shapes work out!

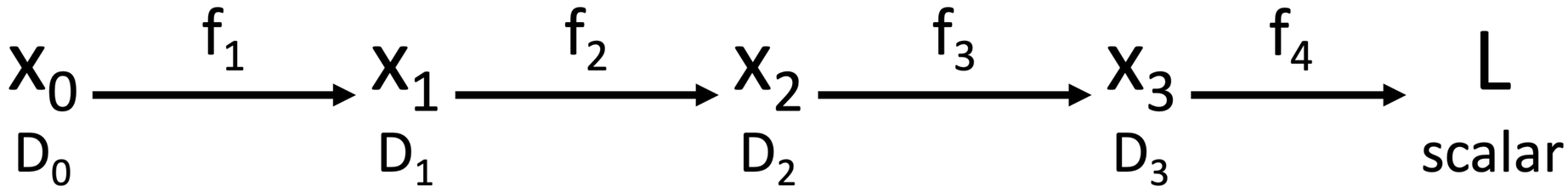
Backpropagation: Another View



Chain rule

$$\frac{\partial L}{\partial x_0} = \left(\frac{\partial x_1}{\partial x_0}\right)\left(\frac{\partial x_2}{\partial x_1}\right)\left(\frac{\partial x_3}{\partial x_2}\right)\left(\frac{\partial L}{\partial x_3}\right)$$

Backpropagation: Another View



Matrix multiplication is **associative**: we can compute products in any order

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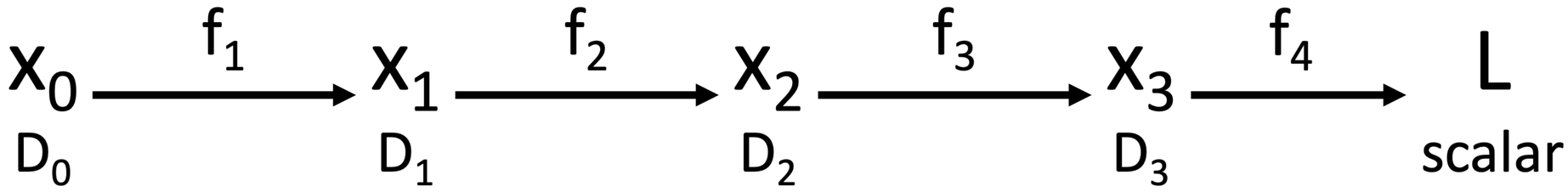
$[D_0 \times D_1]$ $[D_1 \times D_2]$ $[D_2 \times D_3]$ $[D_3]$

Reverse-Mode Automatic Differentiation



Matrix multiplication is **associative**: we can compute products in any order

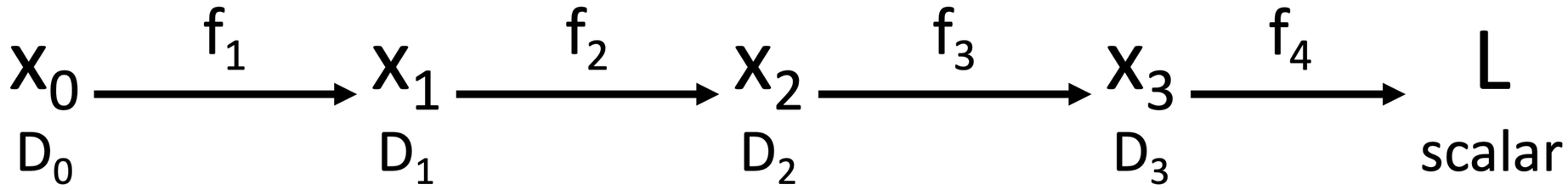
Computing products right-to-left avoids matrix-matrix products; only needs matrix-vector

Chain rule

$$\frac{\partial L}{\partial x_0} = \left(\frac{\partial x_1}{\partial x_0}\right)\left(\frac{\partial x_2}{\partial x_1}\right)\left(\frac{\partial x_3}{\partial x_2}\right)\left(\frac{\partial L}{\partial x_3}\right)$$

$[D_0 \times D_1]$ $[D_1 \times D_2]$ $[D_2 \times D_3]$ $[D_3]$

Reverse-Mode Automatic Differentiation



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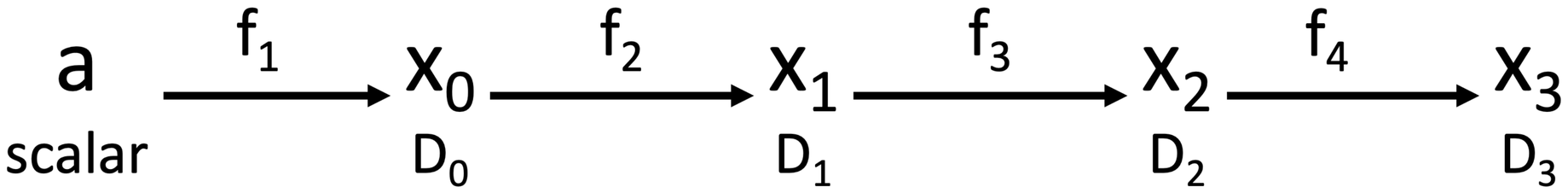
$[D_0 \times D_1]$ $[D_1 \times D_2]$ $[D_2 \times D_3]$ $[D_3]$

Compute grad of scalar output w/respect to all vector inputs

What if we want grads of scalar input w/respect to vector outputs?

Forward-Mode Automatic Differentiation

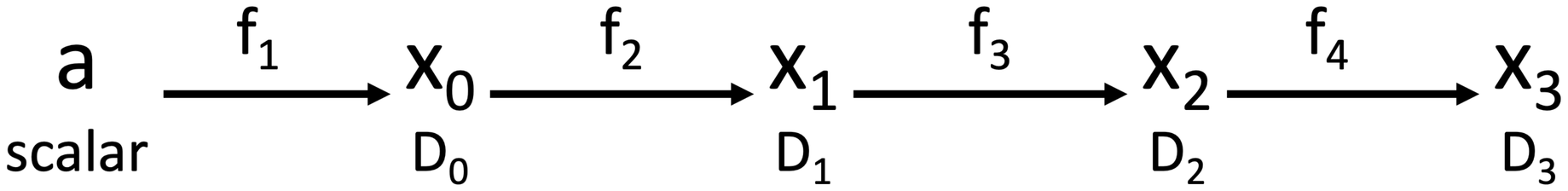


Chain rule

$$\frac{\partial x_3}{\partial a} = \left(\frac{\partial x_0}{\partial a}\right)\left(\frac{\partial x_1}{\partial x_0}\right)\left(\frac{\partial x_2}{\partial x_1}\right)\left(\frac{\partial x_3}{\partial x_2}\right)$$

$[D_0]$ $[D_0 \times D_1]$ $[D_1 \times D_2]$ $[D_2 \times D_3]$

Forward-Mode Automatic Differentiation



Computing products left-to-right avoids matrix-matrix products; only needs matrix-vector

Chain rule

$$\frac{\partial x_3}{\partial a} = \left(\frac{\partial x_0}{\partial a}\right)\left(\frac{\partial x_1}{\partial x_0}\right)\left(\frac{\partial x_2}{\partial x_1}\right)\left(\frac{\partial x_3}{\partial x_2}\right)$$

$[D_0]$ $[D_0 \times D_1]$ $[D_1 \times D_2]$ $[D_2 \times D_3]$

Universal Approximation

A neural network with one hidden layer can approximate any function $f: \mathbb{R}^N \rightarrow \mathbb{R}^M$ with arbitrary precision*

*Many technical conditions: Only holds on compact subsets of $\mathbb{R}^N$; function must be continuous; need to define "arbitrary precision"; etc.

Universal Approximation

Let $\phi(\cdot)$ be a non-constant, bounded and monotone-increasing continuous function. Let I_{m_0} denote the m_0-dimensional unit hypercube $[0, 1]^{m_0}$. The space of continuous functions on I_{m_0} is denoted by $C(I_{m_0})$. Then, given any function $f \in C(I_{m_0})$ and $\epsilon > 0$, there exists an integer m_1 and sets of real constants α_i, β_i, and w_{ij}, where $i = 1, \ldots, m_1$ and $j = 1, \ldots, m_0$ such that we may define

$$F(x_1, \ldots, x_{m_0}) = \sum_{i=1}^{m_1} \alpha_i \phi \left(\sum_{j=1}^{m_0} w_{ij} x_j + b_i \right)$$

as an approximation realization of the function $f(\cdot)$: that is,

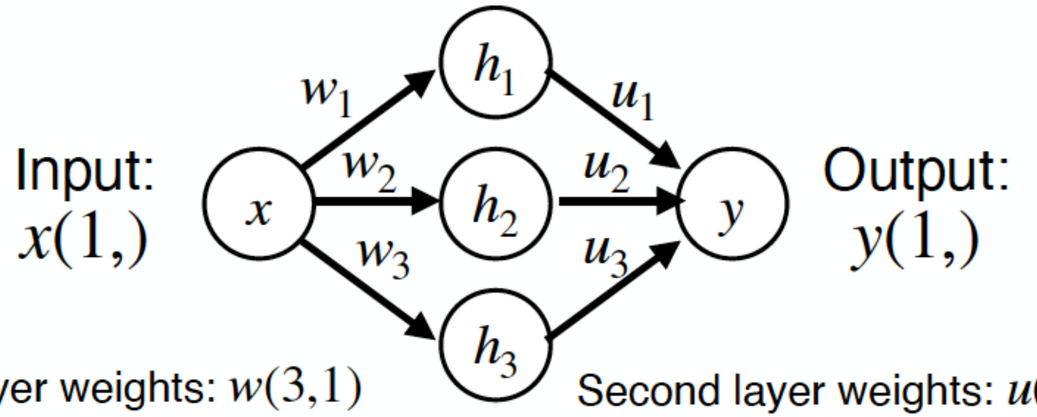
$$|F(x_1, \ldots, x_{m_0}) - f(x_1, \ldots, x_{m_0})| < \epsilon$$

for all $x_1, x_2, \ldots, x_{m_0}$ in the input space.

- Essentially, the Universal Approximation Theorem states that a single hidden layer is sufficient for a multilayer perceptron to compute a uniform ϵ approximation to a given training set - provided you have the *right* number of neurons and the *right* activation function.
  (However, this does not say that a single hidden layer is optimal with regards to learning time, generalization, etc.)

Universal Approximation

Example: Approximating a function $f: \mathbb{R} \to \mathbb{R}$ with a two-layer ReLU network



First layer weights: $w(3,1)$

First layer bias: $b(3,)$

Second layer weights: $u(3,1)$

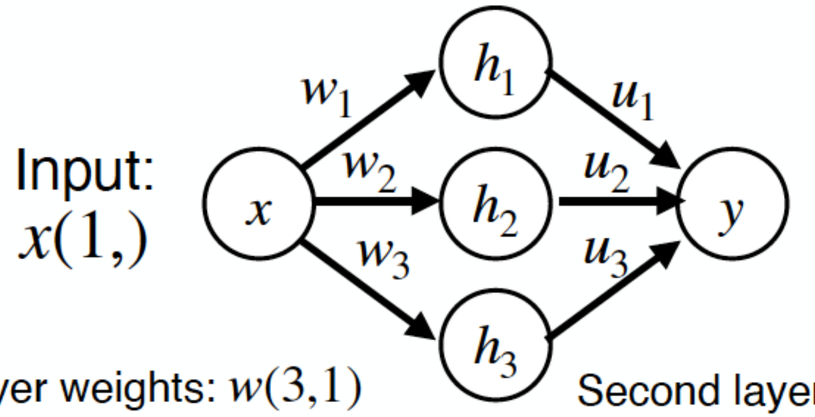
First layer bias: $p(1,)$

$$h_1 = \max(0, w_1 x + b_1)$$
$$h_2 = \max(0, w_2 x + b_2)$$
$$h_1 = \max(0, w_3 x + b_3)$$
$$y = u_1 h_1 + u_2 h_2 + u_3 h_3 + p$$

$$y = u_1 \max(0, w_1 x + b_1) + u_2 \max(0, w_2 x + b_2) + u_3 \max(0, w_3 x + b_3) + p$$

Universal Approximation

Example: Approximating a function $f: \mathbb{R} \to \mathbb{R}$ with a two-layer ReLU network



First layer weights: $w(3,1)$

First layer bias: $b(3,)$

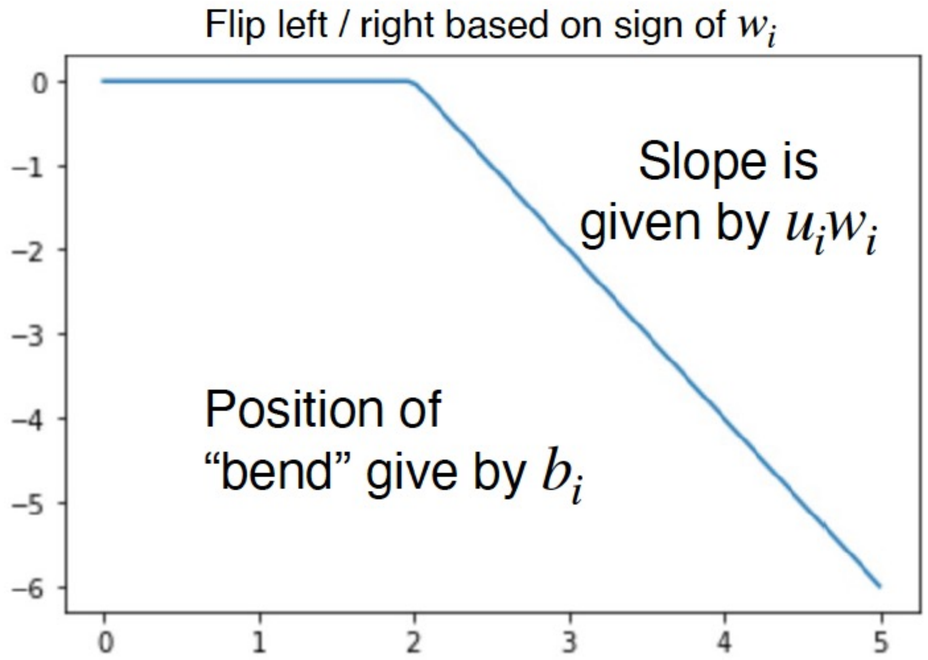
Second layer weights: $u(3,1$

First layer bias: $p(1,)$

$$h_1 = \max(0, w_1 x + b_1)$$
$$h_2 = \max(0, w_2 x + b_2)$$
$$h_1 = \max(0, w_3 x + b_3)$$
$$y = u_1 h_1 + u_2 h_2 + u_3 h_3 + p$$

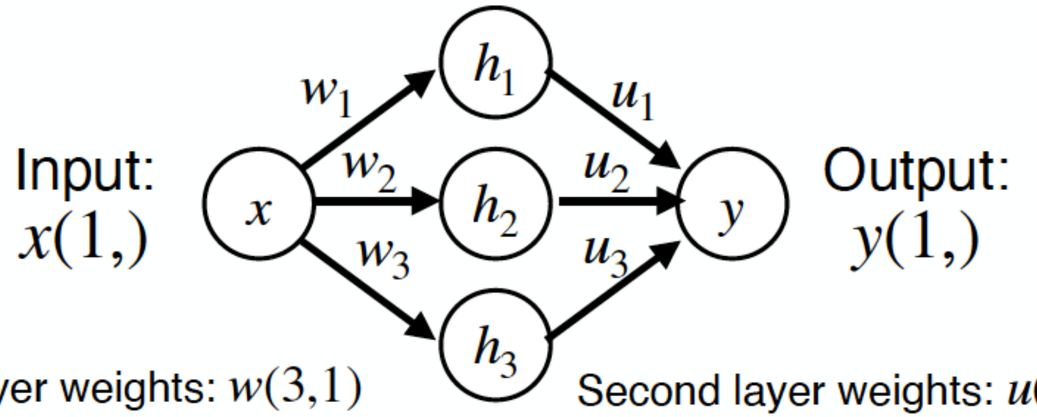
$$y = u_1 \max(0, w_1 x + b_1) + u_2 \max(0, w_2 x + b_2) + u_3 \max(0, w_3 x + b_3) + p$$

Output is a sum of shifted, scaled ReLUs:



Universal Approximation

Example: Approximating a function $f: \mathbb{R} \to \mathbb{R}$ with a two-layer ReLU network



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$$h_1 = \max(0, w_1 x + b_1)$$
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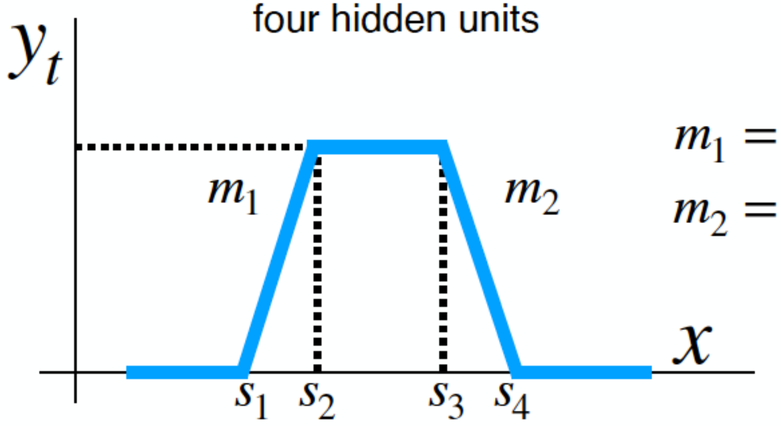
$$h_1 = \max(0, w_3 x + b_3)$$
$$y = u_1 h_1 + u_2 h_2 + u_3 h_3 + p$$

$$y = u_1 \max(0, w_1 x + b_1) + u_2 \max(0, w_2 x + b_2) + u_3 \max(0, w_3 x + b_3) + p$$

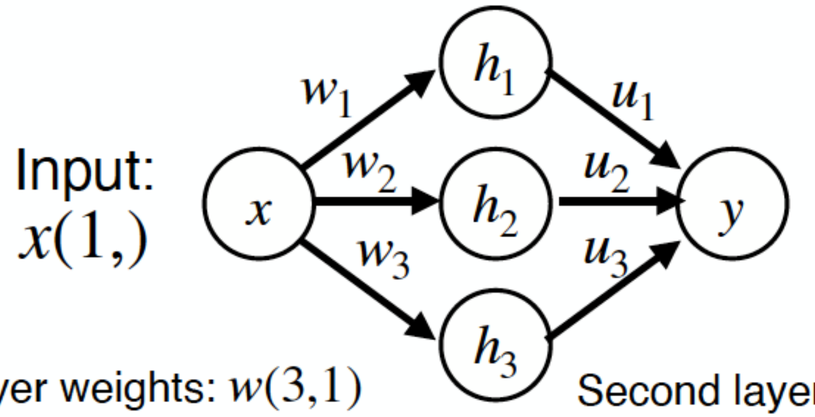
We can build a "bump function" using four hidden units



$$m_1 = t/(s_2 - s_1)$$
$$m_2 = t/(s_4 - s_3)$$

Universal Approximation

Example: Approximating a function $f: \mathbb{R} \to \mathbb{R}$ with a two-layer ReLU network



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$$y = u_1 h_1 + u_2 h_2 + u_3 h_3 + p$$

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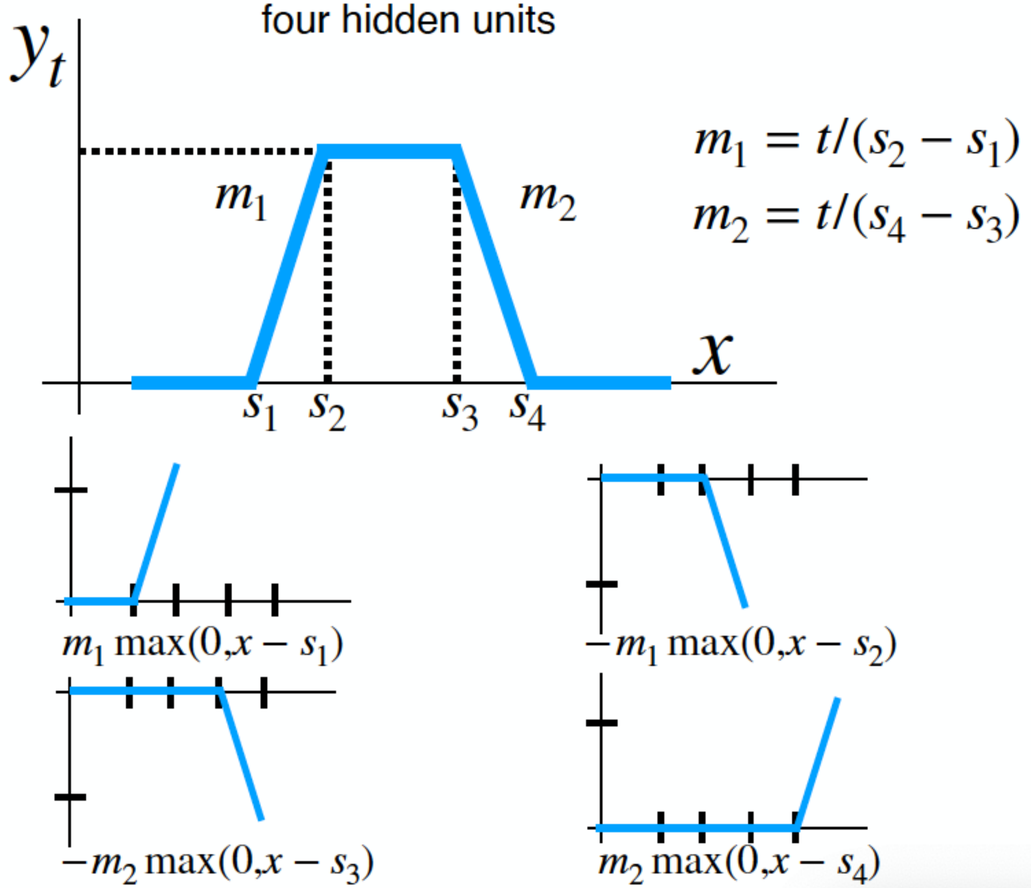
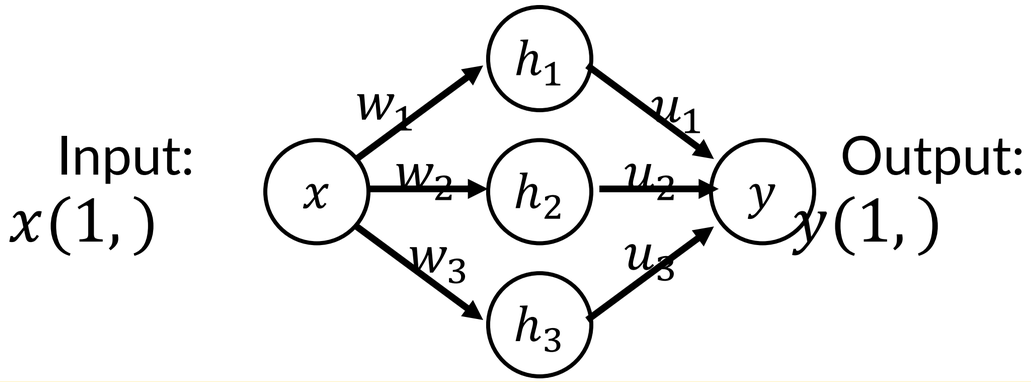
We can build a "bump function" using four hidden units



Universal Approximation

Example: Approximating a function $f: \mathbb{R} \to \mathbb{R}$ with a two-layer ReLU network



Universal approximation tells us:

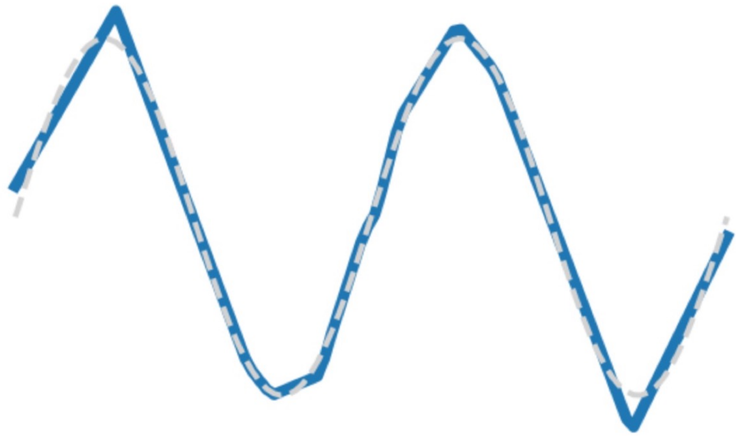
- Neural nets can represent any function

Universal approximation DOES NOT tell us:

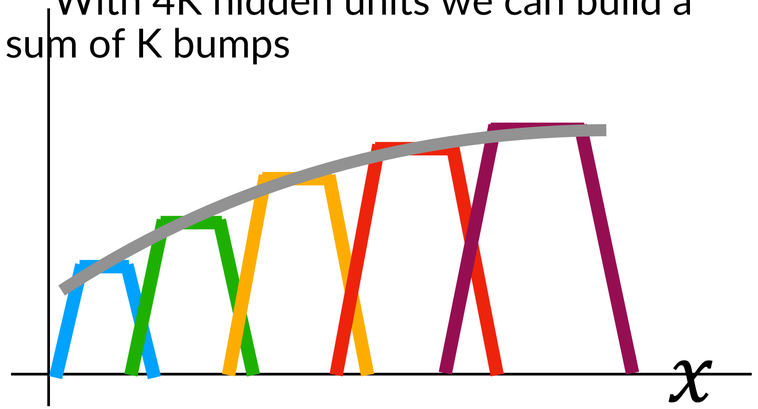
- Whether we can actually learn any function with SGD
- How much data we need to learn a function

Remember: kNN is also a universal approximator!

Reality check: Networks don't really learn bumps!



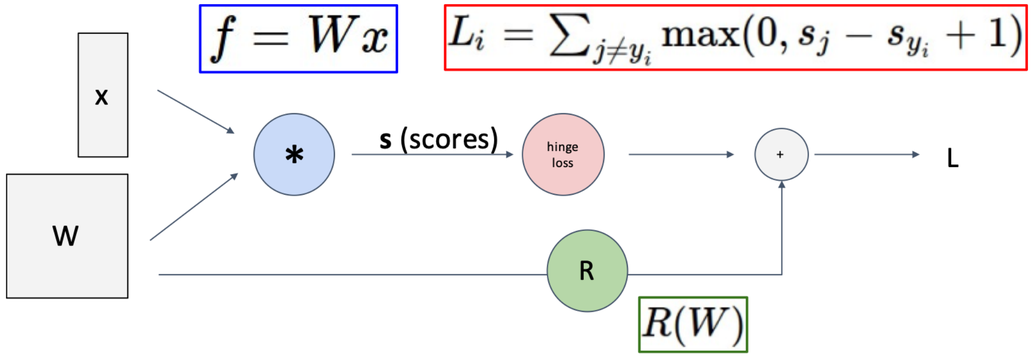
With 4K hidden units we can build a sum of K bumps



Approximate functions with bumps!

Summary

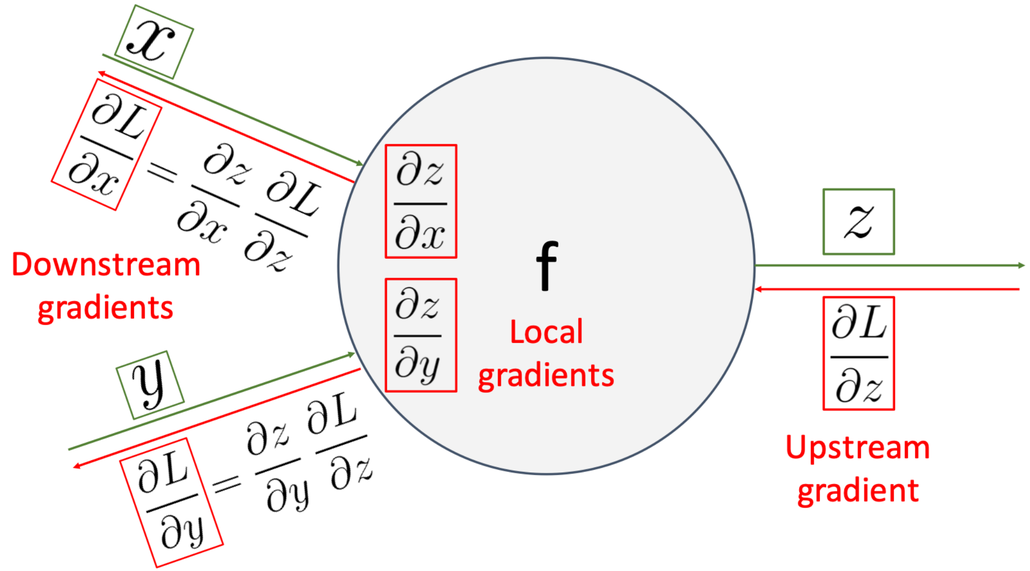
Represent complex expressions as **computational graphs**



Forward pass computes outputs

Backward pass computes gradients

During the backward pass, each node in the graph receives **upstream gradients** and multiplies them by **local gradients** to compute **downstream gradients**



Summary

Backprop can be implemented with “flat” code where the backward pass looks like forward pass reversed (Use this for A2!)

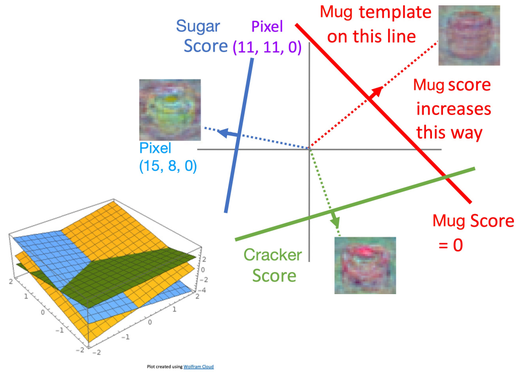
```
def f(w0, x0, w1, x1, w2):
  s0 = w0 * x0
  s1 = w1 * x1
  s2 = s0 + s1
  s3 = s2 + w2
  L = sigmoid(s3)

  grad_L = 1.0
  grad_s3 = grad_L * (1 - L) * L
  grad_w2 = grad_s3
  grad_s2 = grad_s3
  grad_s0 = grad_s2
  grad_s1 = grad_s2
  grad_w1 = grad_s1 * x1
  grad_x1 = grad_s1 * w1
  grad_w0 = grad_s0 * x0
  grad_x0 = grad_s0 * w0
```

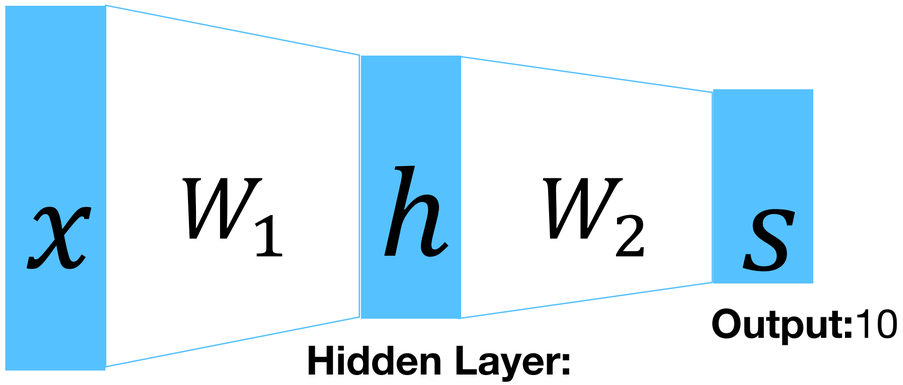
Backprop can be implemented with a modular API, as a set of paired forward/backward functions

```
class Multiply(torch.autograd.Function):
  @staticmethod
  def forward(ctx, x, y):
    ctx.save_for_backward(x, y)
    z = x * y
    return z
  @staticmethod
  def backward(ctx, grad_z):
    x, y = ctx.saved_tensors
    grad_x = y * grad_z   # dz/dx * dL/dz
    grad_y = x * grad_z   # dz/dy * dL/dz
    return grad_x, grad_y
```

Summary



$$f(x) = W_2 max(0, W_1 x + b_1) + b_2$$

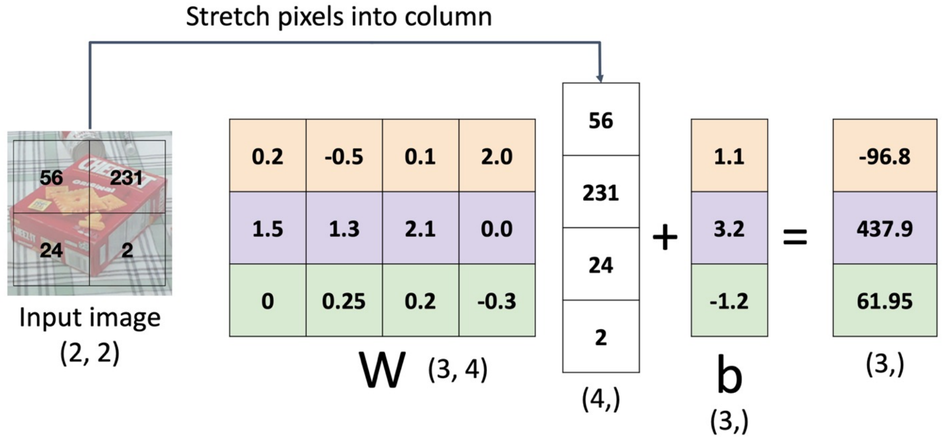


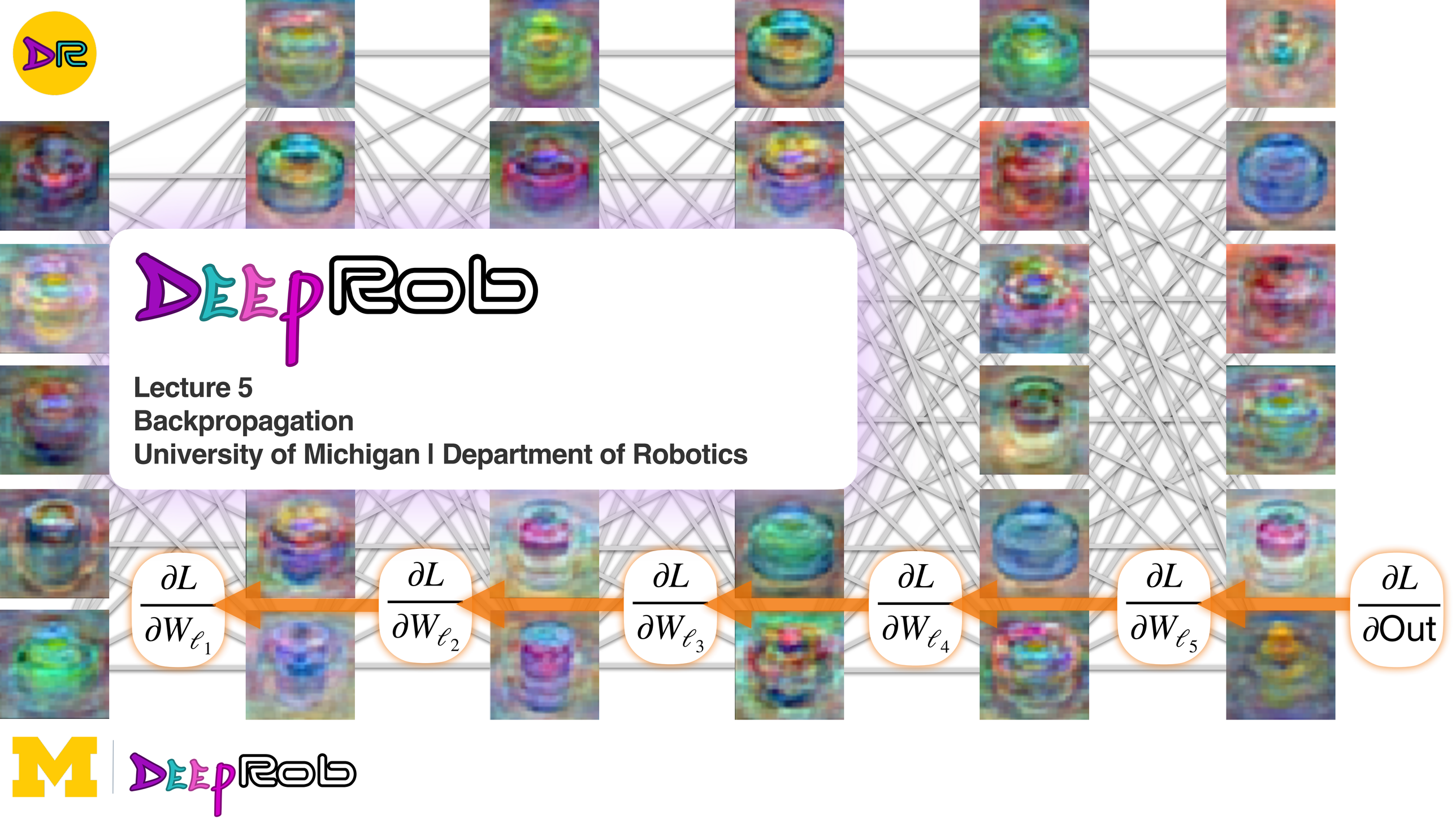
Input:
3072

Hidden Layer:
100

Output:10

Problem: So far our classifiers don't respect the spatial structure of images!




DEEPROB
Lecture 5
Backpropagation
University of Michigan | Department of Robotics
$\frac{\partial L}{\partial W_{\ell_1}}$
$\frac{\partial L}{\partial W_{\ell_2}}$
$\frac{\partial L}{\partial W_{\ell_3}}$
$\frac{\partial L}{\partial W_{\ell_4}}$
$\frac{\partial L}{\partial W_{\ell_5}}$
$\frac{\partial L}{\partial \text{Out}}$
DEEPROB